Institute of Mathematics and Computer Science European Bioinformatics Institute

AIMS User Guide

Version 2.10

Accessing AIMS system

To access Assay 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. If user has access to several Technologies, his access rights for different Technologies might be different.

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

Changing user settings

User settings page allows to modify a number of user-specific settings. The modified values are activated immediately in the current session as well as saved and used in subsequent sessions. The settings that currently can be modified are the following:

Page size. This value specifies the number of entries that are displayed in single page in either of *1st level (Views)*, *2nd level (Samples)*, *3rd level (Assays)* pages. The default value (if not modified by user) depends from the configuration of particular AIMS instance.

Start with welcome page. This specifies whether after login in the system the first page that is displayed is "Welcome page". The main purpose of this page is showing which user group is used as *default group* in current session, and consequently, what access rights other users will have to entries created by user within a particular session.

Default user group. This allows to change a user group that will be used as as *default* in current session, and consequently, what access rights other users will have to entries created within this particular session. The access rights specific to the selected *default group* are shown in table below.

Change password. Allows user to change password.

Welcome page

Welcome page can be displayed as a first page after login in the system. Whether this is the case depends from the settings of user account and can be modified by user by clicking on *User settings* tab. In addition, the page will be unconditionally displayed to users with administrator rights if there are some external tasks that need to be performed.

The main functionality of this page is the option to see and change if necessary the *default group* that will be used in current session, and consequently, what access rights other users will have to entries created within this particular session. The access rights specific to the selected *default group* are shown in table below.

Study level

List of Studies page allows to view/edit/delete data either for all Studies currently in database, which are attributed to particular Technology, or Studies contained within a particular View (if Views are configured for the given Technology). If your access rights don't allow to access a particular Experiment even in *view only* mode, only the value of Study ID will be shown, all other values will be replaced by **.

Selection of Technology

If no Technology is selected, as a first step you must select a particular Technology you will be working with. To do this, click on *Select Technology* tab, select a Technology from drop-down list and click on *Change* button. Technology can be changed at later stage using *Select Technology* tab. Note that when Technology is changed all settings made for this Technology during the current session (such that configurations of Views/Study/Assays pages or filter settings) are lost.

Creating/viewing/editing/deleting Studies

- To add a new Study to database click on *New Study* tab. If you are viewing Studies attributed to one particular Study then new Study will be defined for that group. Otherwise the new Study will be created together with a new Study.

- To edit data about a Study click on the corresponding edit icon ${\Bbb S}$. If you have limited

access rights one of the following icons will be shown instead: 5 (the Edit dialog is available in *view only* mode, you can also view data and supplementary files for the particular Study),

(the Edit dialog is available in *view only* mode, you cannot access data and supplementary files), (you don't have access to Study).

- To create a new Study with the parameters copied from the existing one click on the corresponding *clone* icon \heartsuit . If you don't have access rights to a particular Study, the icon will be replaced by \heartsuit .

- To delete entry about a particular Study click on the corresponding *edit* icon and then press *Delete* button. If there are Assays attributed to the given Study the button will be replaced with * *Delete*. This allows deleting of Study and **all** Assays belonging to it. Since this is a potentially dangerous operation, you will need to reconfirm the intention to delete as well as to provide the exact number of Assays belonging to this Study.

- To change simultaneously the values of some properties for several Studies click on *Batch edit* tab. You will have the option to select Studies for editing and then, after pressing *Edit Selected* button, will be directed to edit dialog which allows to change properties of selected Studies.

Add/Edit/View Study dialog allows you correspondingly to enter data about a new Study or to edit/view (depending of your access rights) data for already existing Study.

The values of *Study Ids* are generated automatically, these values depend from Technology and user who is creating Study. Ids of Studies are unique.

Data files and Supplementary files allow you to link to Study and upload data files obtained from experiments as well as supplementary information files. Depending from AIMS configuration you have the option of just uploading files from your local computer, or choice between uploading files from your local computer or selection of files already pre-uploaded via FTP. Depending from technology configuration you also may have the option to associate *file type* with each of the files, however currently this is treated just as informal comment. It is possible to link several Data or Supplementary files with each Study, however you need to press *Update* button after linking each of the files and re-open Edit dialog for linking another one.

Technically there is no difference between treatment of *Data files* and *Supplementary files*, however it is recommended that *Data files* are used for files obtained from experiments and *Supplementary files* for providing additional information which can't be entered via Edit dialog fields.

The meaning of other fields hopefully should be self-apparent. The datatypes for each of the fields are shown on the right side (position mouse over datatype names for some additional information).

In *Batch edit* mode there is a checkbox for each of Studies' fields. Check the boxes for fields values of which you wish to change. Fields are displayed in white, if its values for all Studies selected for batch editing is the same, and gray if there are different values. *Name* fields cannot be changed in *Batch edit* mode.

Navigation

To navigate to **List of Assays** page showing Assays of a particular Study click on

Associating Studies with Views

This functionality is available if Views are configured for the given Technology and Studies associated with a particular View are currently listed.

To change which Studies are includes in a given View click on *Define View* tab. All Studies will be listed with a checkbox on a right side (checked for Studies belonging to the given View). You can freely modify the values of checkboxes and either click on *OK Define View* (the Studies associated with this View will be redefined) or on link *Cancel Define View* (the previous set of Studies for this View will be kept).

Batch edit

In *Batch edit* mode there is a checkbox for each of entries' fields. Check the ones you wish to change for all entries in the batch. The fields left unchecked (displayed gray) can hold different values for each entry and the checked ones (displayed white) will hold the changed value for all entries.

Batch uploading

Upload 1st level (Studies) page allows to upload multiple entries from a single tabdelimited file. The file must contain a header row with recognized column names (these consist of a level prefix followed by ".", "Parameter group" (defined in *Parameters* table) and the value corresponding to "Upload name" field in in *Parameters* table - e.g. *Study.Software details.Version*) followed by rows corresponding to uploadable entries. Upload names of fields that are configured in (defined in *Common parameters* table) are not configurable in *Common parameters* table, but specified in "systemConst.xml" file (and in future will be shown in this table in read-only mode). Usually these names consist only of two components, e.g. *Study.ID*. Also, there is extended syntax options for columns describing uploadable files (see below). Level prefixes (e.g. *View, Study, Assay*) are also specified in specified in "systemConst.xml" file.

To obtain a correct header for a particular level, you can download tab-delimited files containing only this header by clicking on *Download … header* or *Download … header* (*minimal*) links; these will provide correspondingly either a header containing all recognized column names, or a "minimal" header containing only names of mandatory columns.

There are three "checkbox" options that you can select for batch uploads at all levels:

- Generate identifiers automatically. If checked, automatic id generation of IDs will be

used and the corresponding column, e.g. Studies.ID, either ignored or disallowed (depending from *Allow unrecognized columns* setting. ID generation will not work at 1st level (View), if the ID generation at this level is not configured for a particular Technology. If unchecked, column with IDs (e.g. Study.ID) is mandatory and it is required that IDs must be unique (but see the next option).

- **Allow duplicate rows**. If checked, then entries with identical IDs are allowed in upload file, however only a single (assume that randomly selected) entry will be uploaded in system. Generally this option could be useful only in combination with unselected *Generate identifiers automatically* and selected *Allow unrecognized columns*. The expected use case is uploading a single file containing entries of all three levels - in this case the "whole collection" can be uploaded by uploading the same file correspondingly at 1st, 2nd and 3rd level.

- **Allow unrecognized columns**. If checked, the upload file can contain arbitrary column names that are not recognized by the system. The most typical usage could be uploading a file with columns for all three AIMS levels (most of them of recognized only at their own level, apart from parent level ID, which could be used also at child level).

In addition, at 2nd and 3rd levels there is a radio button allowing to specify one of the following options:

- uploading all entries as child entries for parent entry shown (and selectable) in listbox; - uploading each entry by specifying its own parent by its ID. In this case a column with parent ID must be present in upload file (e.g. when uploading 3rd level entries (Assays) the file must contain also column *Study.ID*);

- uploading each entry by specifying its own parent by its NAME. In this case a column with parent NAME must be present in upload file (e.g. when uploading 3rd level entries (Assays) the file must contain also column *Study.NAME*).

At 2nd level (*Studies*) there is also a checkbox **Upload under view** that activates/deactivates radio button area. If deactivated, the entries will not be made children of any 1st level entry. Note that whilst there is many-to-many relationship between 1st and 2nd level entries, via data upload it is possible to make a 2nd level entry a child only of one 1st level entry.

Locations of upload files.

In all situations the page will contain the following two *Browse* buttons:

- **Parameter file**. This allows you to browse your local file system and select tab-delimited file for upload.

- **Local zipped data**. This allows to provide a zipped archive containing all the files that are referenced in parameter file (if any). This ZIP archive is also uploaded form your local file system. Whilst technically this is a simplest option for file upload, http protocol might impose severe limitation of archive size that can be uploaded in this way.

If the system *and* you access rights are configured for pre-uploading files via FTP, two additional options will be provided:

- **FTP zipped data**. Instead of uploading ZIP archive from your local system, you can browse for archives that are already pre-uploaded on the server.

- **FTP directory**. This provides a similar pre-uploading option, however in this case you have to specify a pre-uploaded directory containing all the referenced files. This option may be more convenient for very large files that are hard to pack in a single archive. A notable difference from the previous option is that in this case you *shouldn't reference the same file more than once*. Ignoring this will result in a partially corrupt upload, requiring substantial manual correction!

If data/supplementary files are pre-uploaded via FTP, there will be some delay before Assays will be available for editing (Ξ will be shown instead of edit icon). (Edit dialogs still will be available for users with administrator rights, although note that data files still will not be

copied into repository and changing file references are likely to cause errors.) If icon \mathbb{Z} is shown, this means that there have been some problems with copying data and supplementary files.

Referencing data and supplementary files.

The column names in header for referencing files that have to be uploaded are defined in "systemConst.xml" file and will be shown in complete header obtainable via *Download* ... *header* link. E.g., the column names might be *Study.DATA_F*, *Study.DF_TYPE* for data files, and *Study.SUPPL_F*, *Study.SF_TYPE* for supplementary (protocol) files. The following features have to be taken into account:

- columns for data or supplementary files will only be available (or recognized), if linking of files to entries is configured for particular Collection and particular level;

- the file name (given e.g. in *Study.DATA_F*) must contain a full path to file either in ZIP archive or in pre-uploaded directory.

- the file type (given e.g. in *Study.DF_TYPE*) is a memo field describing the file. The list of recognized values can be checked in Edit dialog that corresponds to uploaded entries (there could be none).

- there is extended syntax allowing to upload multiple files for a single entry. The names of columns that reference files can contain additional suffix of the form *#file_number*, where "file_number" is an arbitrary string which distinguishes different columns. E.g. to upload two files for a single entry two columns either headers *Study.DATA_F#1*, *Study.DATA_F#2*, or headers *Study.DATA_F#SS*, *Study.DATA_F#17* could be used. The same suffixes can be used to specify corresponding file types, e.g. *Study.DF_TYPE#1*, *Study.DF_TYPE#2*.

Data Export and Transfer

Both data and metadata export (i.e. request made by user's specifications) and data/metadata transfer (predefined export to a particular) data warehouse are accessible from the same tab *Data export/transfer*. To access it from *Views/Studies/Assays view pages*, first click on *Export* tab, select the entries you wish to export and click on *Data export/transfer* tab. Depending from technology configuration and your access rights a page with a nonempty subset from the following three sections will be displayed.

Data transfer (transfer name)

This allows to transfer selected entries to data warehouse for which such transfer is configured for particular technology. Usually each entry should be transfered just once, thus transfered entries are flagged and although a repeated transfer of flagged entries is possible, a warning will be issued before doing so.

Note that configuration of data transfer for a given technology makes this option available only from a single AIMS level (either from *Views*, *Studies* or *Assays*.

The only configurable option in this section is a field for entering email - in this case the processing program will send the updates of processing status of transfers to this address. Apart from that, a list of configuration files used for metadata transfer as well as a list of transferred higher level entries (with number of their children) are shown (depending from the configuration a transfer may include either metadata or datafile transfer or both).

There is a choice to request transfer by pressing *Transfer* button and cancelling the operation. When transfer has been requested the corresponding entries will be marked for processing and files will be transferred later by an external program. The following flags will be used to

mark entries: 🏂 (transfer has been requested), 🏂 (the actual transfer of data has been

successfully completed), 🗣 (a successful reception of data has been confirmed), 👎 (either the actual data transfer has failed, or data warehouse has reported that there are problems

with transferred files). Some of these flags may not be available for soma data transfer configurations.

Metadata export

This allows to export metadata according to configuration that is specified by XML template. According from you access rights there may be only option to select from *Configuration files* provided by system administrator, or also an option to *Upload your own configuration file*. The syntax of configuration file is described in a separate document, but it allows to configure meta data export in XML file in rather flexible format. Export can include metadata from the aims AIMS level from which it has been requested, from all child levels as well as from all SIMS levels that are referenced from these entries.

Export file can be generated in two formats: XML (native format) and TSV (a tab delimited file that is obtained from "flattening" native XML file).

Data export

This allows to export data and supplementary files. For the option to functional you must additionally setup the options how the data files will be delivered. This is done via XML configuration file that should be set up by system administrator.

There are two options how transfers is being made (and these should be specified in configuration file mentioned above): sending of files to FTP to a server of your choice (in this case you should provide to administrator server location and login details), and copying files on the same server to different directory (e.g. your account home directory). The configurable options in this section are: providing *Export name* (this should be obtained from administrator and will be used to recognize that export is initiated by you and ned to be delivered to your location) and email address for feedback (an email will be sent to this address after the export will be completed). After the export is requested, the corresponding entries will be marked for processing and files will be exported later by an external program.

Directories of XML configuration files

The root directory of configuration files is defined in *web.xml* file by *<context-param>* entry data_transfer_configuration.directory. Within this directory the location of configuration files are as follows:

Metadata export configuration files:

exports/[technology directory]/l1 (export at Assays level), exports/[technology directory]/l2 (export at Studies level), exports/[technology directory]/l3 (export at Views level), where [technology directory] is defined by FTP directory entry in **Technologies** table.

Date transfer configuration files:

transfers/[technology directory]/[transfer directory], where *[technology directory]* is defined as above and *[transfer directory]* corresponds to *Data directory* entry in **Transfer types** table.

Assay level

List of Assays page allows to view/edit/delete data either for all Assays currently in database, which are attributed to particular Technology, or Assays attributed to particular Experiment. If your access rights don't allow to access a particular Assay even in view only mode, only the value of Assay ID will be shown, all other values will be replaced by **.

Selection of Technology

If no Technology is selected, as a first step you must select a particular Technology you will be working with. To do this, click on Select Technology tab, select a Technology from drop-down list and click on *Change* button. Technology can be changed at later stage using the same Select Technology tab. Note that when Technology is changed all settings made for this Technology during the current session (such that configurations of Study/Experiment/Assay pages or filter settings) are lost.

Creating/viewing/editing/deleting Assays

- To add a new Assay to database click on New Assay tab. If you are viewing Assays attributed to one particular Experiment then new Assay will be defined for that group. Otherwise the new Assay will be created together with a new Experiment.

- To edit data about a Assay click on the corresponding *edit* icon \mathbb{I} . 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 can also view data and supplementary files for the particular Assay),

(the Edit dialog is available in *view only* mode, you cannot access data and supplementary

files), (you don't have access to Assay). - To create a new Assay with the parameters copied from the existing one click on the

corresponding *clone* icon \heartsuit . If you don't have access rights to a particular Assay, the icon will be replaced by 🔌

- To delete entry about a particular Assay click on the corresponding edit icon ${\mathbb F}$ and then press Delete button.

- To change simultaneously the values of some properties for several Assays click on Batch edit tab. You will have the option to select Assays for editing and then, after pressing Edit Selected button, will be directed to edit dialog which allows to change properties of selected Assays.

Add/Edit/View Assay dialog allows you correspondingly to enter data about a new Assay or to edit/view (depending of your access rights) data for already existing Assay.

The values of Assay Ids are generated automatically, these values depend from Technology, Experiment and user who is creating Assay. Ids of Assays attributed to a particular Experiment will be unique.

The Aliquot field should either be filled by using the prompting button (if available) and selecting the referenced Aliquot from the list (in case when multiple Aliquots will be selected, several Assays, one for each Aliquot, will be created); or can be filled with arbitrary string value (including empty) if prompting button is unavailable. The requirement of Aliquot prompting depends from AIMS configuration.

Data files and Supplementary files allow you to link to Assay and upload data files obtained from experiments as well as supplementary information files. Depending from AIMS configuration you have the option of just uploading files from your local computer, or choice between uploading files from your local computer or selection of files already pre-uploaded via FTP. Depending from technology configuration you also may have the option to associate file

type with each of the files, however currently this is treated just as informal comment. It is possible to link several Data or Supplementary files with each Assay, however you need to press *Update* button after linking each of the files and re-open Edit dialog for linking another one.

Technically there is no difference between treatment of *Data files* and *Supplementary files*, however it is recommended that *Data files* are used for files obtained from experiments and *Supplementary files* for providing additional information which can't be entered via Edit dialog fields.

The meaning of other fields hopefully should be self-apparent. The datatypes for each of the fields are shown on the right side (position mouse over datatype names for some additional information).

Batch edit

In *Batch edit* mode there is a checkbox for each of Assays' fields. Check the boxes for fields values of which you wish to change. Fields are displayed in white, if its values for all Assays selected for batch editing is the same, and gray if there are different values. *Name* and *Aliquot* fields cannot be changed in *Batch edit* mode.

Batch uploading

Upload Assays page allows to upload multiple entries from a single tab-delimited file. The file must contain a header row with recognized column names (these consist of a level prefix followed by ".", "Parameter group" (defined in *Parameters* table) and the value corresponding to "Upload name" field in in *Parameters* table - e.g. *Study.Software details.Version*) followed by rows corresponding to uploadable entries. Upload names of fields that are configured in (defined in *Common parameters* table) are not configurable in *Common parameters* table, but specified in "systemConst.xml" file (and in future will be shown in this table in read-only mode). Usually these names consist only of two components, e.g. *Study.ID*. Also, there is extended syntax options for columns describing uploadable files (see below). Level prefixes (e.g. *View, Study, Assay*) are also specified in "systemConst.xml" file.

To obtain a correct header for a particular level, you can download tab-delimited files containing only this header by clicking on *Download … header* or *Download … header* (*minimal*) links; these will provide correspondingly either a header containing all recognized column names, or a "minimal" header containing only names of mandatory columns.

There are three "checkbox" options that you can select for batch uploads at all levels:

- *Generate identifiers automatically*. If checked, automatic id generation of IDs will be used and the corresponding column, e.g. Studies.ID, either ignored or disallowed (depending from *Allow unrecognized columns* setting. ID generation will not work at 1st level (View), if the ID generation at this level is not configured for a particular Technology. If unchecked, column with IDs (e.g. Study.ID) is mandatory and it is required that IDs must be unique (but see the next option).

- **Allow duplicate rows**. If checked, then entries with identical IDs are allowed in upload file, however only a single (assume that randomly selected) entry will be uploaded in system. Generally this option could be useful only in combination with unselected *Generate identifiers automatically* and selected *Allow unrecognized columns*. The expected use case is uploading a single file containing entries of all three levels - in this case the "whole collection" can be uploaded by uploading the same file correspondingly at 1st, 2nd and 3rd level.

- **Allow unrecognized columns**. If checked, the upload file can contain arbitrary column names that are not recognized by the system. The most typical usage could be uploading a file with columns for all three AIMS levels (most of them of recognized only at their own level, apart from parent level ID, which could be used also at child level).

In addition, at 2nd and 3rd levels there is a radio button allowing to specify one of the

following options:

- uploading all entries as child entries for parent entry shown (and selectable) in listbox; - uploading each entry by specifying its own parent by its ID. In this case a column with parent ID must be present in upload file (e.g. when uploading 3rd level entries (Assays) the file must contain also column *Study.ID*);

- uploading each entry by specifying its own parent by its NAME. In this case a column with parent NAME must be present in upload file (e.g. when uploading 3rd level entries (Assays) the file must contain also column *Study.NAME*).

At 2nd level (*Studies*) there is also a checkbox **Upload under view** that activates/deactivates radio button area. If deactivated, the entries will not be made children of any 1st level entry. Note that whilst there is many-to-many relationship between 1st and 2nd level entries, via data upload it is possible to make a 2nd level entry a child only of one 1st level entry.

Locations of upload files.

In all situations the page will contain the following two *Browse* buttons:

- **Parameter file**. This allows you to browse your local file system and select tab-delimited file for upload.

- **Local zipped data**. This allows to provide a zipped archive containing all the files that are referenced in parameter file (if any). This ZIP archive is also uploaded form your local file system. Whilst technically this is a simplest option for file upload, http protocol might impose severe limitation of archive size that can be uploaded in this way.

If the system *and* you access rights are configured for pre-uploading files via FTP, two additional options will be provided:

- **FTP zipped data**. Instead of uploading ZIP archive from your local system, you can browse for archives that are already pre-uploaded on the server.

- **FTP directory**. This provides a similar pre-uploading option, however in this case you have to specify a pre-uploaded directory containing all the referenced files. This option may be more convenient for very large files that are hard to pack in a single archive. A notable difference from the previous option is that in this case you *shouldn't reference the same file more than once*. Ignoring this will result in a partially corrupt upload, requiring substantial manual correction!

If data/supplementary files are pre-uploaded via FTP, there will be some delay before Assays

will be available for editing ($\stackrel{\scriptstyle imes}{\scriptstyle imes}$ will be shown instead of edit icon). (Edit dialogs still will be available for users with administrator rights, although note that data files still will not be

copied into repository and changing file references are likely to cause errors.) If icon \mathbb{Z} is shown, this means that there have been some problems with copying data and supplementary files.

Referencing data and supplementary files.

The column names in header for referencing files that have to be uploaded are defined in "systemConst.xml" file and will be shown in complete header obtainable via *Download* ... *header* link. E.g., the column names might be *Study.DATA_F*, *Study.DF_TYPE* for data files, and *Study.SUPPL_F*, *Study.SF_TYPE* for supplementary (protocol) files. The following features have to be taken into account:

- columns for data or supplementary files will only be available (or recognized), if linking of files to entries is configured for particular Collection and particular level;

- the file name (given e.g. in *Study.DATA_F*) must contain a full path to file either in ZIP archive or in pre-uploaded directory.

- the file type (given e.g. in *Study.DF_TYPE*) is a memo field describing the file. The list of recognized values can be checked in Edit dialog that corresponds to uploaded entries (there could be none).

- there is extended syntax allowing to upload multiple files for a single entry. The names of columns that reference files can contain additional suffix of the form *#file_number*, where "file_number" is an arbitrary string which distinguishes different columns. E.g. to upload two files for a single entry two columns either headers *Study.DATA_F#1*, *Study.DATA_F#2*, or headers *Study.DATA_F#SS*, *Study.DATA_F#17* could be used. The same suffixes can be used to specify corresponding file types, e.g. *Study.DF_TYPE#1*, *Study.DF_TYPE#2*.

Data Export and Transfer

Both data and metadata export (i.e. request made by user's specifications) and data/metadata transfer (predefined export to a particular) data warehouse are accessible from the same tab *Data export/transfer*. To access it from *Views/Studies/Assays view pages*, first click on *Export* tab, select the entries you wish to export and click on *Data export/transfer* tab. Depending from technology configuration and your access rights a page with a nonempty subset from the following three sections will be displayed.

Data transfer (transfer name)

This allows to transfer selected entries to data warehouse for which such transfer is configured for particular technology. Usually each entry should be transfered just once, thus transfered entries are flagged and although a repeated transfer of flagged entries is possible, a warning will be issued before doing so.

Note that configuration of data transfer for a given technology makes this option available only from a single AIMS level (either from *Views*, *Studies* or *Assays*.

The only configurable option in this section is a field for entering email - in this case the processing program will send the updates of processing status of transfers to this address. Apart from that, a list of configuration files used for metadata transfer as well as a list of transferred higher level entries (with number of their children) are shown (dpending from the configuration a transfer may include either metadata or datafile transfer or both). There is a choice to request transfer by pressing *Transfer* button and cancelling the operation.

When trasfer has been requested the corresponding entries will be marked for processing and files will be transfered later by an external program. The following flags will be used to mark

entries: 🔊 (transfer has been requested), 🎾 (the actual transfer of data has been

successfully completed), 🗭 (a successful reception of data has been confirmed), 🗭 (either the actual data transfer has failed, or data warehouse has reported that there are problems with transferred files). Some of these flags may not be available for soma data transfer configurations.

Metadata export

This allows to export metadata according to configuration that is specified by XML template. According from you access rights there may be only option to select from *Configuration files* provided by system administrator, or also an option to *Upload your own configuration file*. The syntax of configuration file is described in a separate document, but it allows to configure meta data export in XML file in rather flexible format. Export can include metadata from the aims AIMS level from which it has been requested, from all child levels as well as from all SIMS levels that are referenced from these entries.

Export file can be generated in two formats: XML (native format) and TSV (a tab delimited file that is obtained from "flattening" native XML file).

Data export

This allows to export data and supplementary files. For the option to functional you must

additionally setup the options how the data files will be delivered. This is done via XML configuration file that should be set up by system administrator.

There are two options how tranbfers is being made (and these should be specified in configuration file mentioned above): sending of files bu FTP to a server of your choice (in this case you should provide to administrator server location and login details), and copying files on the same server to different directory (e.g. your account home directory). The configurable options in this section are: providing *Export name* (this should be obtained from administrator and will be used to recognize that export is initiated by you and ned to be delivered to your location) and emaila ddress for feedback (an email will be sent to this address after the export will be completed). After the export is requested, the corresponding entries will be marked for processing and files will be exported later by an external program.

Directories of XML configuration files

The root directory of configuration files is defined in *web.xml* file by *<context-param>* entry data_transfer_configuration.directory. Within this directory the location of configuration files are as follows:

Metadata export configuration files:

exports/[technology directory]/l1 (export at Assays level), exports/[technology directory]/l2 (export at Studies level), exports/[technology directory]/l3 (export at Views level), where [technology directory] is defined by FTP directory entry in **Technologies** table.

Date transfer configuration files:

transfers/[technology directory]/[transfer directory], where *[technology directory]* is defined as above and *[transfer directory]* corresponds to *Data directory* entry in **Transfer types** table.

View level

List of Views page allows to view/edit/delete data either for all Views currently in database, which are attributed to particular Technology. This page is available only if Views are configured for the given Technology. If your access rights don't allow to access a particular View even in *view only* mode, only the value of View ID will be shown, all other values will be replaced by **.

There is an important difference between *Views* and *Studies/Assays* levels. Whilst there is a hierarchical *one-to-many* relation between *Studies* and *Assays* - each *Assay* belongs to exactly one *Study* and will be deleted, if that *Study* will be deleted, there are possible *many-to-many* relations between *Views* and *Studies* are not affected by creation or deletion of Views. The association between *Views* and *Studies* are defined from **List of Views** page. For more information see *First level (Studies) help page*.

Selection of Technology

Generally **List of Views** is available only if a technology is already selected. Technology can be changed at later stage using the same *Select Technology* tab, selecting a Technology from drop-down list and clicking on *Change* button. Note that when Technology is changed all settings made for this Technology during the current session (such that configurations of Views/Studies/Assays pages or filter settings) are lost.

Creating/viewing/editing/deleting Views

- To add a new View to database click on New View tab.

- To edit data about a View click on the corresponding *edit* icon \mathbb{I} . If you have limited access

rights one of the following icons will be shown instead: 6 (the Edit dialog is available in *view*

only mode, you can also view data and supplementary files for the particular View), Edit dialog is available in *view only* mode, you cannot access data and supplementary files),

(you don't have access to View).

- To create a new View with the parameters copied from the existing one click on the

corresponding *clone* icon \bigotimes . If you don't have access rights to a particular View, the icon will be replaced by \bigotimes .

- To delete entry about a particular View click on the corresponding *edit* icon $\stackrel{[s]}{=}$ and then press *Delete* button. If there are Assays attributed to the given View the button will be replaced with * *Delete*. This allows deleting of View and **all** Assays belonging to it. Since this is a potentially dangerous operation, you will need to reconfirm the intention to delete as well as to provide the exact number of Assays belonging to this View.

Add/Edit/View View dialog allows you correspondingly to enter data about a new View or to edit/view (depending of your access rights) data for already existing View.

The values of *View Ids* are generated automatically, these values depend from Technology and user who is creating View. Ids of Views are unique.

Data files and Supplementary files allows you to link to View and upload data files obtained from Views as well as supplementary information files. Depending from AIMS configuration you have the option of just uploading files from your local computer, or choice between uploading files from your local computer or selection of files already pre-uploaded via FTP. Depending from technology configuration you also may have the option to associate *file type* with each of the files, however currently this is treated just as informal comment. It is possible to link several Data or Supplementary files with each View, however you need to press *Update* button after linking each of the files and re-open Edit dialog for linking another one.

Technically there is no difference between treatment of *Data files* and *Supplementary files*, however it is recommended that *Data files* are used for files obtained from Views and *Supplementary files* for providing additional information which can't be entered via Edit dialog fields.

The meaning of other fields hopefully should be self-apparent. The datatypes for each of the fields are shown on the right side (position mouse over datatype names for some additional information).

Navigation

To navigate to **List of Studies** page showing Studies associated with a particular View click on icon.

Batch edit

In *Batch edit* mode there is a checkbox for each of entries' fields. Check the ones you wish to change for all entries in the batch. The fields left unchecked (displayed gray) can hold different values for each entry and the checked ones (displayed white) will hold the changed value for all entries.

Batch upload

Upload Views page allows to upload multiple entries from a single tab-delimited file. The file must contain a header row with recognized column names (these consist of a level prefix followed by ".", "Parameter group" (defined in *Parameters* table) and the value corresponding to "Upload name" field in in *Parameters* table - e.g. *Study.Software details.Version*) followed by rows corresponding to uploadable entries. Upload names of fields that are configured in (defined in *Common parameters* table) are not configurable in *Common parameters* table, but specified in "systemConst.xml" file (and in future will be shown in this table in read-only mode). Usually these names consist only of two components, e.g. *Study.ID*. Also, there is extended syntax options for columns describing uploadable files (see below). Level prefixes (e.g. *View, Study, Assay*) are also specified in "systemConst.xml" file.

To obtain a correct header for a particular level, you can download tab-delimited files containing only this header by clicking on *Download … header* or *Download … header* (*minimal*) links; these will provide correspondingly either a header containing all recognized column names, or a "minimal" header containing only names of mandatory columns.

There are three "checkbox" options that you can select for batch uploads at all levels:

- *Generate identifiers automatically*. If checked, automatic id generation of IDs will be used and the corresponding column, e.g. Studies.ID, either ignored or disallowed (depending from *Allow unrecognized columns* setting. ID generation will not work at 1st level (View), if the ID generation at this level is not configured for a particular Technology. If unchecked, column with IDs (e.g. Study.ID) is mandatory and it is required that IDs must be unique (but see the next option).

- **Allow duplicate rows**. If checked, then entries with identical IDs are allowed in upload file, however only a single (assume that randomly selected) entry will be uploaded in system. Generally this option could be useful only in combination with unselected *Generate identifiers automatically* and selected *Allow unrecognized columns*. The expected use case is uploading a single file containing entries of all three levels - in this case the "whole collection" can be uploaded by uploading the same file correspondingly at 1st, 2nd and 3rd level.

- **Allow unrecognized columns**. If checked, the upload file can contain arbitrary column names that are not recognized by the system. The most typical usage could be uploading a file with columns for all three AIMS levels (most of them of recognized only at their own level, apart from parent level ID, which could be used also at child level).

In addition, at 2nd and 3rd levels there is a radio button allowing to specify one of the following options:

- uploading all entries as child entries for parent entry shown (and selectable) in listbox; - uploading each entry by specifying its own parent by its ID. In this case a column with parent ID must be present in upload file (e.g. when uploading 3rd level entries (Assays) the file must contain also column *Study.ID*);

- uploading each entry by specifying its own parent by its NAME. In this case a column with parent NAME must be present in upload file (e.g. when uploading 3rd level entries (Assays) the file must contain also column *Study.NAME*).

At 2nd level (*Studies*) there is also a checkbox **Upload under view** that activates/deactivates radio button area. If deactivated, the entries will not be made children of any 1st level entry. Note that whilst there is many-to-many relationship between 1st and 2nd level entries, via data upload it is possible to make a 2nd level entry a child only of one 1st level entry.

Locations of upload files.

In all situations the page will contain the following two *Browse* buttons:

- **Parameter file**. This allows you to browse your local file system and select tab-delimited file for upload.

- **Local zipped data**. This allows to provide a zipped archive containing all the files that are referenced in parameter file (if any). This ZIP archive is also uploaded form your local file system. Whilst technically this is a simplest option for file upload, http protocol might impose severe limitation of archive size that can be uploaded in this way.

If the system *and* you access rights are configured for pre-uploading files via FTP, two additional options will be provided:

- **FTP zipped data**. Instead of uploading ZIP archive from your local system, you can browse for archives that are already pre-uploaded on the server.

- **FTP directory**. This provides a similar pre-uploading option, however in this case you have to specify a pre-uploaded directory containing all the referenced files. This option may be more convenient for very large files that are hard to pack in a single archive. A notable difference from the previous option is that in this case you *shouldn't reference the same file more than once*. Ignoring this will result in a partially corrupt upload, requiring substantial manual correction!

If data/supplementary files are pre-uploaded via FTP, there will be some delay before Assays

will be available for editing (\succeq will be shown instead of edit icon). (Edit dialogs still will be available for users with administrator rights, although note that data files still will not be

copied into repository and changing file references are likely to cause errors.) If icon $\overset{\scriptstyle{\scriptstyle{\Delta}}}{=}$ is shown, this means that there have been some problems with copying data and supplementary files.

Referencing data and supplementary files.

The column names in header for referencing files that have to be uploaded are defined in "systemConst.xml" file and will be shown in complete header obtainable via *Download* ... *header* link. E.g., the column names might be *Study.DATA_F*, *Study.DF_TYPE* for data files, and *Study.SUPPL_F*, *Study.SF_TYPE* for supplementary (protocol) files. The following features have to be taken into account:

- columns for data or supplementary files will only be available (or recognized), if linking of files to entries is configured for particular Collection and particular level;

- the file name (given e.g. in Study.DATA_F) must contain a full path to file either in ZIP

archive or in pre-uploaded directory.

- the file type (given e.g. in *Study.DF_TYPE*) is a memo field describing the file. The list of recognized values can be checked in Edit dialog that corresponds to uploaded entries (there could be none).

- there is extended syntax allowing to upload multiple files for a single entry. The names of columns that reference files can contain additional suffix of the form *#file_number*, where "file_number" is an arbitrary string which distinguishes different columns. E.g. to upload two files for a single entry two columns either headers *Study.DATA_F#1*, *Study.DATA_F#2*, or headers *Study.DATA_F#SS*, *Study.DATA_F#17* could be used. The same suffixes can be used to specify corresponding file types, e.g. *Study.DF_TYPE#1*, *Study.DF_TYPE#2*.

Data Export and Transfer

Both data and metadata export (i.e. request made by user's specifications) and data/metadata transfer (predefined export to a particular) data warehouse are accessible from the same tab *Data export/transfer*. To access it from *Views/Studies/Assays view pages*, first click on *Export* tab, select the entries you wish to export and click on *Data export/transfer* tab. Depending from technology configuration and your access rights a page with a nonempty subset from the following three sections will be displayed.

Data export

This allows export of multiple data/supplementary files. The files from all selected entries (as well as their descendants) will be sent to a specified ftp account. You must provide such information as: *Name of ftp server*, *Name of ftp account*, *Password for this ftp account* (if required) and *Directory name on ftp server to which data will be transferred* (optional) as well as *email address for feedback* (optional, if used this is the address to which information about processing of this export request will be sent). There is also an option to test ftp connection with parameters you have provided (click on button *Test connection*). The connection parameters can be saved for repeated use - if you click on button *Save connection*, the parameters you entered will be available as default when *Data export* dialog will be accessed the next time (these data are associated with your account and are not shared with other users.). After the export is requested, the corresponding entries will be marked for processing and files will be exported later by an external program; in addition to these files an xml file containing list of transferred files will be saved in your ftp directory. After the processing of requested export a confirmation email will be sent (if an email address has been entered).

Metadata export

This allows to export metadata according to configuration that is specified by XML template. According from you access rights there may be only option to select from *Configuration files* provided by system administrator, or also an option to *Upload your own configuration file*.

The syntax of configuration file is described in a separate document, but it allows to configure meta data export in XML file in rather flexible format. Export can include metadata from the aims AIMS level from which it has been requested, from all child levels as well as from all SIMS levels that are referenced from these entries.

Export file can be generated in two formats: XML (native format) and TSV (a tab delimited file that is obtained from "flattening" native XML file)

Data transfer (transfer name)

This allows to transfer selected entries to data warehouse for which such transfer is configured for particular technology. Usually each entry should be transfered just once, thus transfered entries are flagged and although a repeated transfer of flagged entries is possible, a warning will be issued before doing so. Note that configuration of data transfer for a given technology makes this option available only from a single AIMS level (either from *Views*, *Studies* or *Assays*.

The only configurable option in this section is a field for entering email - in this case the processing program will send the updates of processing status of transfers to this address. Apart from that, a list of configuration files used for metadata transfer as well as a list of transferred higher level entries (with number of their children) are shown (dpending from the configuration a transfer may include either metadata or datafile transfer or both).

There is a choice to request transfer by pressing *Transfer* button and cancelling the operation. When trasfer has been requested the corresponding entries will be marked for processing and files will be transfered later by an external program. The following flags will be used to mark

entries: Detrimination (transfer has been requested), Detrimination (the actual transfer of data has been

successfully completed), (a successful reception of data has been confirmed), (either the actual data transfer has failed, or data warehouse has reported that there are problems with transferred files). Some of these flags may not be available for soma data transfer configurations.

Directories of XML configuration files

The root directory of configuration files is defined in *web.xml* file by *<context-param>* entry data_transfer_configuration.directory. Within this directory the location of configuration files are as follows:

Metadata export configuration files: exports/[technology directory]/l1 (export at Assays level), exports/[technology directory]/l2 (export at Studies level), exports/[technology directory]/l3 (export at Views level), where [technology directory] is defined by FTP directory entry in **Technologies** table.

Date transfer configuration files:

transfers/[technology directory]/[transfer directory], where *[technology directory]* is defined as above and *[transfer directory]* corresponds to *Data directory* entry in **Transfer types** table.

Data filtering

Filter settings page allows to search for Study Groups/Assays with values of selected fields equal to the values defined in search page filters.

The fields, which are available for filtering, are defined in **parameters** and **common_parameters** tables. To define a filter for a particular field, enter a filtering expression for this field. The syntax of filtering expressions is as follows:

- symbol "%" matches any substring (including empty substrings),
- symbol "_" matches any single symbol,
- all other symbols match themselves.

The filtering is done by SQL queries and for some particular datatypes (boolean, lists of numbers, etc.) the syntax of "right" filtering expressions may not be intuitive. For fields of fixed vocabulary types a drop-down list is provided instead of filtering expression.

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.

To display all database entries press *Cancel filter* button either on Study Groups or on Assays page.

Defining tabular views and reports

Configure columns

Configure ... columns page allows to select which columns and in which order will be displayed in View, Study or Assay 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 **Configure ... columns** 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 **Configure ... columns** 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).

Reports

This is the simplest way of data export, providing export of Studies in WYSIWYG mode. By clicking on Report button you are able to save the data shown on Study page in tab-delimited format. Included in the report are the same columns that are currently configured as visible in Study page (see Column configuration). In the report you will get only the data you have permission to view. You can manage the data you wish to include in your report either by using filter first or by clicking on the "Export" link first and manually selecting the entries you wish to see in the report. In both cases, the report will contain all selected data, even if the entries are on several pages and not visible. Check the number of items on top of the list (next to "Uncheck all" button if in batch export mode).

Vocabulary tables

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

Vocabularies that are available for editing depends from currently selected technology. Shown are vocabularies that are defined for the particular technology (this is done in **Configuration tables** page) as well as *common* vocabularies that are available for all technologies (these are defined separately in **Administrator tables** page).

Editing options include adding new entries to the vocabulary, deleting existing entries, renaming existing entries and changing the order in which entries will be available for selection. To add a new entry click on a *new* link for a specific vocabulary. To edit/delete entry

click on *edit* icon \mathbb{I} for a specific vocabulary. To change the display order use correspondingly ∇ and \triangle icons.

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. However changing the order in which entries are displayed for selection is safe operation in such context and doesn't affect the data already stored in the system.

The length of vocabulary tables is limited by a 4000 character long encoding of vocabulary in database.

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

Request technology

If you have the rights to request a technology, you should be able to find the **Request technology** link in your *user settings* page. **Request technology** page allows to send an email with an xml file containing desired technology configuration to your AIMS instance administrator. You should enter the email of your administrator in the first field.

Technology name is the name that will be visible in the *technology list* for users that will be allowed to access it when the administrator imports it into the AIMS instance.

Use as template allows you to use one of technologies available to you as a template configuration to make changes to.

You have three levels (Views, studies, Assays) in which you can manipulate parameters. You can add new parameters, you can change the order of the added parameters (using the green arrows on the right), you can delete them and edit them. You can edit:

Long name - shows up next to a parameter field in edit page.

Short name - shows up on top of the column in view page.

Upload name - determines the name of that parameter column in "upload entries" file.

Parameter group - parameters can be grouped for more structure. Parameter groups are visible in view page.

Parameter type - the type of data you wish to store. For text chose *bigstring*, for "yes / no" chose *boolean*, for real numbers chose *float* and you can chose *integer* or one of the kinds of *date* available. For parameters that you wish to have predefined values that can be selected from a listbox, chose *TABLE* and specify the values you wish to have for each of the parameters that you chose *TABLE* for. The administrator will have to enter these manually.

Is required - check this if you think that every entry should have some value for this parameter.

Show in filter - check this if you think that entries could be filtered by this parameter value.

You can write in **Comment** any additional concerns you have, and ways to contact you.

Technology configuration

Configuration tables page allows to access and (depending from your access rights) modify configuration of currently selected technology. The tables shown on this page and their meaning are described below.

Table Parameter types

Contains data types that are available for the current Technology for use in configurable parameter fields. There are 10 base types, some of which may be parametrized by different values of 2 attributes (currently, only Attribute 1 values is used practice). In database all these datatypes are encoded in 200 byte character strings, which places some restrictions on range of values that can be used in these data types. The available base types are:

- string string of up to 200 characters, shown in one line in edit dialogs,

- **bigstring** string of up to 200 characters, shown in multiple lines in edit dialogs,

- **number** integer (range likely depends from what is recognized as integers by java),

- float float (range likely depends from what is recognized as floats by java),

- **boolean** yes/no, represented by checkbox in edit pages,

- **array of number** list of 1 to 10 integers, shown adjacently in one row in edit pages, number of integers given as value for Attribute 1,

- **array of float** list of 1 to 10 floats, shown adjacently in one row in edit pages, of integers given as value for Attribute 1,

- **table**, values from controlled vocabulary defined in **Vocabularies** or **Common Vocabularies** tables (the last can be found on **Administrator tables** page), the required table should be selected in field *Table name*. Values from vocabularies are shown in edit dialogs as drop-down lists.

- **datatime** data and time (if Attribute 1 value is 3), date (if Attribute 1 value is 2) or year (if Attribute 1 value is 1).

- **time** time (duration) in format mm:ss if Attribute 1 value is 3), hh:mm (if Attribute 1 value is 6) or hh:mm:ss (if Attribute 1 value is 7)

The table automatically lists all entries present in **Common parameter types** table (shown on **Administrator tables** page), which are uneditable. In addition new entries can be created and/or edited for a particular technology. Generally this is needed for creation of new parameters of **table** and **array of...** types. The meaning of the table fields should be apparent.

Table Common parameters

Table contains configuration of fixed datatype fields for current Technology for Views, Studies and Assays. For each of these the following fixed type fields are available - *indentifString* (normally used for Ids, string of up to 200 characters), *visibleName* (normally used for Names, string of up to 200 characters), *comment* (string of up to 4000 characters), *dataFiles* (used for associated data files), *protocolFiles* (used for supplementary files), *creator* (FK to **Users** table), *modifier* (FK to **Users** table), *createDate* (datatime), *modifDate* (datatime) and *aliquotId* (string of up to 200 characters and (optionally) FK to referenced Aliquot). Configuration options include visibility and column and row names in edit dialogs. Note that (apart from aliquotID, which should be used only for Assays) there is exactly one field of each type available for Views, Studies and Assays. The configuration of fields *creator*, *modifier*, *createDate* and *modifDate* is optional.

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

- *Parameter short name* - name shown as column name in **List of Views/Studies/Assays** pages,

- Parameter long name - name shown on the left side of the field in Add/Edit/View dialogs,

- Parameter upload name - name used in header of batch upload file (this is currently provided for reference purposes only - the upload names for common parameters are hard-coded in the

software),,

- Assay column name - the name of field which is configured (doesn't apply to Assays, if left empty),

- *Study column name* - the name of field which is configured (doesn't apply to Studies, if left empty),

- *View column name* - the name of field which is configured (doesn't apply to Views, if left empty),

- Assay view column # - column number in List of Assays page (not shown, if 0),

- *Sortable* - if *true*, the entries in **List of Assays** can be shorted by the values of this parameter,

- Study view column # - column number in List of Studies page (not shown, if 0),

- *Sortable* - if *true*, the entries in **List of Studies** can be shorted by the values of this parameter

- View view column # - column number in List of Views page (not shown, if 0),

- *Sortable* - if *true*, the entries in **List of Views** can be shorted by the values of this parameter,

- Show in filter - if true the parameter will be included in data filter,

- Comment - informal comment.

Table Parameters

Table contains configuration of *Fxxx* fields for current Technology for Views, Studies and Assays. Currently up to 55 fields from *F001* to *F055* are available for Views, Studies and Assays. (to increase this, changes should be made in both, data base and program files). Apart from configuration options what is available for *Common parameters*, additionally "soft" data types used for these fields should be configured (available datatypes are these that are given in *Parameter types* table).

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

- Parameter short name - name shown as column name in List of Views/Studies/Assays pages,

- *Parameter group* - parameter group (see *Parameter groups* table in **Administrator tables** page) to which the parameter belongs. Parameter groups affect the upper level header in **List of Views/Studies/Assays** pages and parameter position in Add/Edit/View dialogs (all parameters from the same group are kept together),

- Parameter type - parameter type from Parameter types table,

- Parameter long name - name shown on the left side of the field in Add/Edit/View dialogs,

- Parameter upload name - name used in header of batch upload file,

- Assay column name - the name of field which is configured (doesn't apply to Assays, if left empty),

- *Study column name* - the name of field which is configured (doesn't apply to Studies, if left empty),

- *View column name* - the name of field which is configured (doesn't apply to Views, if left empty),

- *Required* - if *true* the field can't be left empty,

- Assay view column # - column number in List of Assays page (not shown, if 0),

- *Sortable* - if *true*, the entries in **List of Assays** can be shorted by the values of this parameter,

- Study view column # - column number in List of Studies page (not shown, if 0),

- *Sortable* - if *true*, the entries in **List of Studies** can be shorted by the values of this parameter,

- View view column # - column number in List of Views page (not shown, if 0),

- *Sortable* - if *true*, the entries in **List of Views** can be shorted by the values of this parameter,

- Assay row - order number of the field in Add/Edit/View dialog for Assays (within a parameter group),

- Study row - order number of the field in Add/Edit/View dialog for Studies (within a parameter group),

- View row - order number of the field in Add/Edit/View dialog for Views (within a parameter

group),

- Show in filter if true the parameter will be included in data filter,
- Comment informal comment.

Table Data types

Data types are labels for different types of data files that for current Technology can be associated with Views, Studies and Assays. They are optional and for informal use only - processing of data file doesn't depend from data type used for labelling it. The field *Extension* is used for data transfer purposes only - it specifies extension that will be used for file when being sent to target location.

Table Supplementary types

Supplementary types are labels for different types of supplementary files that for current Technology can be associated with Views, Studies and Assays. They are optional and for informal use only - processing of supplementary file doesn't depend from supplementary type used for labelling it.

Table Vocabularies

Defines controlled vocabularies available for current Technology. The content of these controlled vocabularies is accessible and can be modified from **Vocabularies** page. To use these vocabularies, the corresponding parameter **table** types should be additionally configured also in **Parameter types** table. The dialog for entries contains fields *Table* (the name to be referenced in **Parameter types** table) and *Long name* (the name under which vocabulary is shown in **Vocabularies** page) as well as informal *Comment*.

System administration

Administrative tables page allows to access and (depending from your access rights) modify technology independent configuration tables of the system. Generally these tables can be divided in two groups: user and their access rights management and settings that apply to all technologies. The tables shown on this page and their meaning are described below.

Table *Technologies*

Contains data about currently configured Technologies and allows to create new Technologies and modify the existing ones. There is also an option of Technology import in XML format (when doing the Technology name given in import file will be used unless it is already present, in later case it will be modified to make it unique) as well as for Technology configuration export in XML format. The import/export XML files generally contain information about the particular entry in **Technologies** table as well as full contents of tables in **Vocabularies** and **Configuration** pages for the particular Technology. Due to this importing of Technologies should be done with some caution - if the Technology is undesired and needs to be deleted, the contents of tables in **Vocabularies** and **Configuration** pages largely will need to be deleted manually.

Also, when a new Technology is created, contents of tables *Common parameter types* and *Default common parameters* are copied to configuration of new Technology. The table contains the following fields:

- Technology - Technology name,

- *Id prefix* - a string which will be used as part of Id when creating new Studies or Assays, - *FTP directory* - subdirectory from which data and supplementary files will be listed (if FTP option is enabled for this AIMS configuration),

- *Is public* - if *true*, Technology is visible for all users, otherwise only for users configured in *Technology access rights* table,

- Use ID generation - if true IDs will be generated automatically at all levels, otherwise they can be entered manually (generated IDs will be offered, but can be changed),

- Show Views - if true, View level is available for this Technology,

- *transfer type* - if selected from a list (values are defined in **Transfer types** table), a data and metadata transfer option to a specified data warehouse will be available for this Technology,

- Comment - informal comment.

Table *Transfer types*

Describes data transfers (usually to data warehouses) then can be configured for existing technologies. For transfers to be fully configured, additional configuration (XML file defining transfer location and protocol as well as date encryption/compression parameters and feedback processing) must be set up. For this setup you should contact system administrator. The table contains the following fields:

- *Transfer type* - Transfer type name, used for referring to Transfer when configuring Technology,

- Abbreviation - name that is used by external transfer program, this should correspond to the value in additional XML configuration file,

- Data directory - subdirectory for XML templates that are used to configure metadata export (value should be supplied even if metadata export is not needed),

- Transfer from level - specifies from which level (View, Study, Assay transfer is available),

- Comment - informal comment.

Table Parameter groups

Describes Parameter groups which are the upper level header in List of

Studies/Experiments/Assays pages and parameter position in Add/Edit/View dialogs (all parameters from the same group are kept together). Also largely informal, up to extent the use of default groups provided with AIMS is recommended. The table contains the following fields:

- *Parameter group* - Parameter group name, used in defining Parameter group in **Parameters** table for particular technology,

- Short name - name shown in upper level header in List of Views/Studies/Assays pages,

- *Position in Assay* - the order number of fields of this Parameter group in Add/Edit/View dialog for Assays,

- *Position in Study* - the order number of fields of this Parameter group in Add/Edit/View dialog for Studies,

- *Position in View* - the order number of fields of this Parameter group in Add/Edit/View dialog for Views,

- Comment - informal comment.

Table Common parameter types

Contains data types that are available for the all Technologies for use in configurable parameter fields. There are 10 base types, some of which may be parametrized by different values of 2 attributes (currently, only Attribute 1 values is used practice). In database all these datatypes are encoded in 200 byte character strings, which places some restrictions on range of values that can be used in these data types. The available base types are:

- string string of up to 200 characters, shown in one line in edit dialogs,

- **bigstring** string of up to 200 characters, shown in multiple lines in edit dialogs,

- number integer (range likely depends from what is recognized as integers by java),

- float float (range likely depends from what is recognized as floats by java),

- **boolean** yes/no, represented by checkbox in edit pages,

- **array of number** list of 1 to 10 integers, shown adjacently in one row in edit pages, number of integers given as value for Attribute 1,

- **array of float** list of 1 to 10 floats, shown adjacently in one row in edit pages, of integers given as value for Attribute 1,

- **table**, values from controlled vocabulary defined in **Vocabularies** or **Common Vocabularies** tables (the last can be found on **Administrator tables** page), the required table should be selected in field *Table name*. Values from vocabularies are shown in edit dialogs as drop-down lists.

- **datatime** data and time (if Attribute 1 value is 3), date (if Attribute 1 value is 2) or year (if Attribute 1 value is 1).

- **time** time (duration) in format mm:ss if Attribute 1 value is 3), hh:mm (if Attribute 1 value is 6) or hh:mm:ss (if Attribute 1 value is 7)

The meaning of the table fields should be apparent. The table entries are automatically included in *Parameter types* table in **Configuration** page for all Technologies.

Table Default common parameters

Table is used as a template for **Common Parameters** table in **Configuration** page when a new Technology is created.

Table contains configuration of fixed datatype fields for current Technology for Studies, Experiments and Assays. For each of these the following fixed type fields are available *indentifString* (normally used for Ids, string of up to 200 characters), *visibleName* (normally used for Names, string of up to 200 characters), *comment* (string of up to 4000 characters), *dataFiles* (used for associated data files), *protocolFiles* (used for supplementary files), *creator* (FK to **Users** table), *modifier* (FK to **Users** table), *createDate* (datatime), *modifDate* (datatime), *simsBottomRef*, *simsMiddleRef*,*simsTopRef*, and *simsCollectionName* (referencing entries in SIMS).

Configuration options include visibility and column and row names in edit dialogs. Note that there is exactly one field of each type available for Views, Studies and Assays. Field

simsCollectionName should be configured if and only if at least one of the fields *simsBottomRef, simsMiddleRef,simsTopRef* is configured (for particular level). The configuration of fields *creator, modifier, createDate* and *modifDate* is optional. The table contains the following configurable fields:

- Parameter short name - name shown as column name in List of

Studies/Experiments/Assays pages,

- Parameter long name - name shown on the left side of the field in Add/Edit/View dialogs,

- Parameter upload name - name used in header of batch upload file (this is currently provided for reference purposes only - the upload names for common parameters are hard-coded in the software),

- Assay column name - the name of field which is configured (doesn't apply to Assays, if left empty),

- *Study column name* - the name of field which is configured (doesn't apply to Studies, if left empty),

- View column name - the name of field which is configured (doesn't apply to Views, if left empty),

- Assay view column # - column number in List of Assays page (not shown, if 0),

- *Sortable* - if *true*, the entries in **List of Assays** can be shorted by the values of this parameter,

- Study view column # - column number in List of Studies page (not shown, if 0),

- Sortable - if true, the entries in **List of Studies** can be shorted by the values of this parameter

View view column # - column number in List of Views page (not shown, if 0),

- Sortable - if true, the entries in **List of Views** can be shorted by the values of this parameter,

- Show in filter - if true the parameter will be included in data filter,

- Comment - informal comment.

Table Common vocabularies

Defines controlled vocabularies available for all Technologies. The content of these controlled vocabularies is accessible and can be modified from **Vocabularies** page. To use these vocabularies, the corresponding parameter **table** types should be additionally configured also in **Parameter types** table for each Technology where it is used. The dialog for entries contains fields *Table* (the name to be referenced in **Parameter types** table) and *Long name* (the name under which vocabulary is shown in **Vocabularies** page) as well as informal *Comment*.

Table Project partners

Each user can be associated with zero or one of project partners. Currently this serves a memo purpose only (but can be used when creating reports by external software).

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 are nonaccessible (no access to **AdminTables** page), view only, limited editing (actually meaning almost full access, some configuration printouts and external task tables 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,

- Start with welcome page - if true, Welcome page is shown after login into the system,

- *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,

- *Project partner* - allows to specify entry from *Project partners* table with whom this user is associated; currently memo purpose only,

- 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 Technology access rights

Defines users that can access non-public Technologies. The table contains the following fields:

- User - User to which access is given,

- Technology - Technology for which access is given,

- Can create Study - if true, can create new Studies,

- Can create View - if true, can create new Views (if configured for particular Technology),

- *Vocabulary access rights* - the access level to **Vocabularies** page, options are *non-accessible*, *view only*, *limited editing* (can edit existing entries but not delete them or create new ones) and *full editing*,

- Configuration access rights - the access level to **Configuration** page, options are nonaccessible, view only, limited editing (can edit existing entries but not delete them or create new ones) and full editing,

- Data export rights - specifies, what options of XML template based metadata export is available, options are *non-accessible*, *predefined* (only from XML templates previously set up by system administrator), user defined (upload of own templates is possible),

- *Data file export rights* - if *true*, can access data file export functionality (for this to work additional export configuration must be set up with system administrator),

- *Data transfer rights* - if *true*, can initiate data transfer (if configured for particular Technology),

- Comment - informal comment.

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.

Table Pending tasks

Table shows information about data and protocol files associated with uploaded assays that still have to be uploaded in repository. This table generally is for providing information only - unless system errors have occurred, editing isn't recommended.

Table Pending exports

Table shows information about requested data transfers and exports of data files. These entries still needs to be processed by external program. This table generally is for providing information only - unless system errors have occurred, editing isn't recommended.