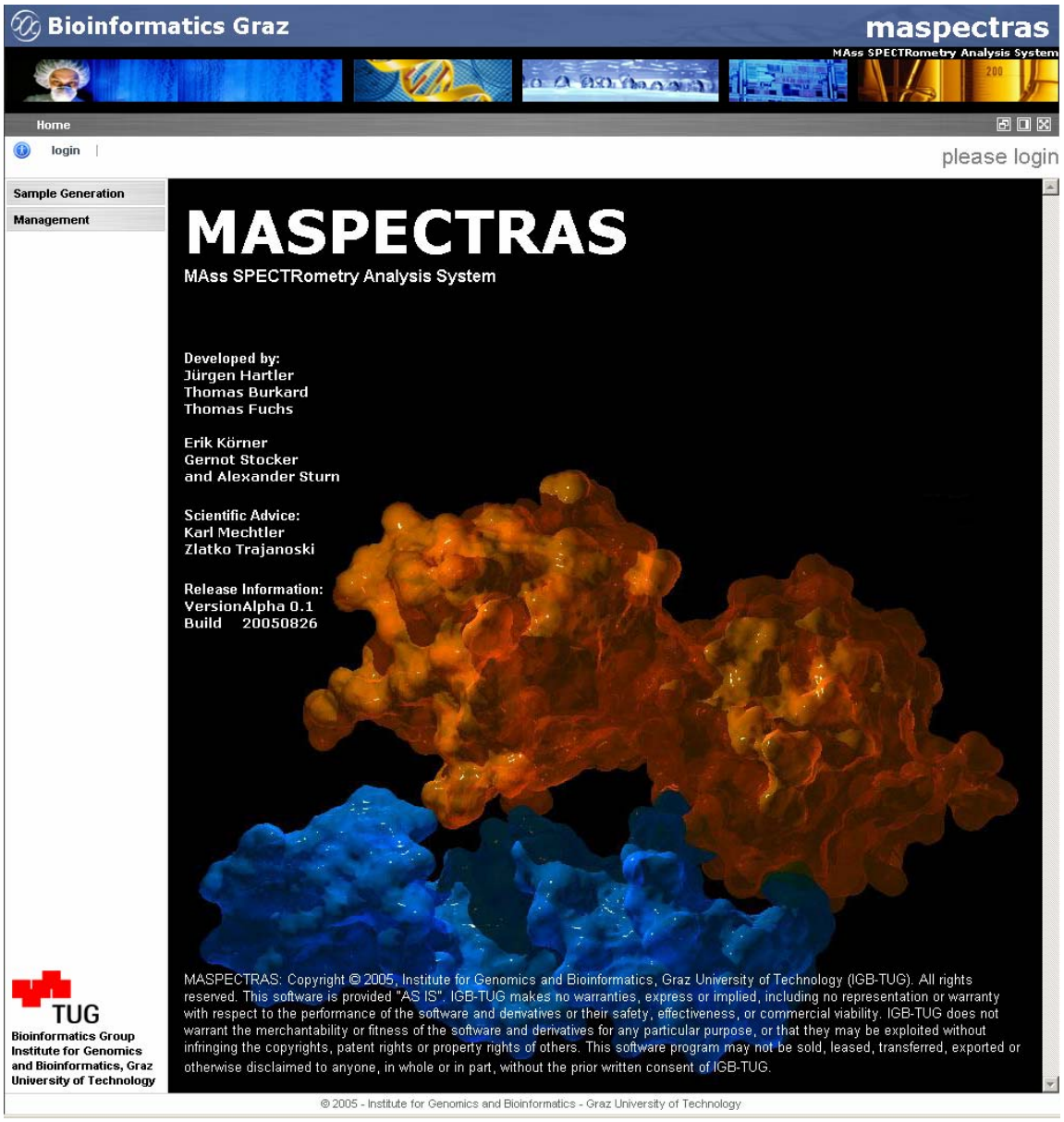
MASPECTRAS

Users Guide

In this user guide every page and functionality is described in detail. To work with MASPECTRAS it is not necessary to read the whole document, because many things work similar to other sections. To work with MASPECTRAS without neglecting any advantages it should be sufficient to read the chapters 1, 2, 6 and 7. The rest should serve as look-up for clarifying ambiguities.

1. General Information:



This will be your first impression of MASPECTRAS.
The main view is divided into 3 sections:

1. The header section consists of some images on the top, of one bar concerning the display and one bar concerning the AAS(Authentication and Authorization System)
2. The left side bar contains the menu
3. The centre frame contains the displayable information

1.1 The header section:

1.1.1 The display bar:

The “Home”-link leads you back to the start page.
At the right side there are 3 icons where you can change the spatial usage of the browser window:

 : brings the window back to the normal size (default setting)

 : with this link you can use the full width of your screen for displaying the information section

 : uses the full width of the window and the images at the header section disappear, only the display bar and the AAS bar will stay.

1.1.2 The display bar:

If you are not logged in:

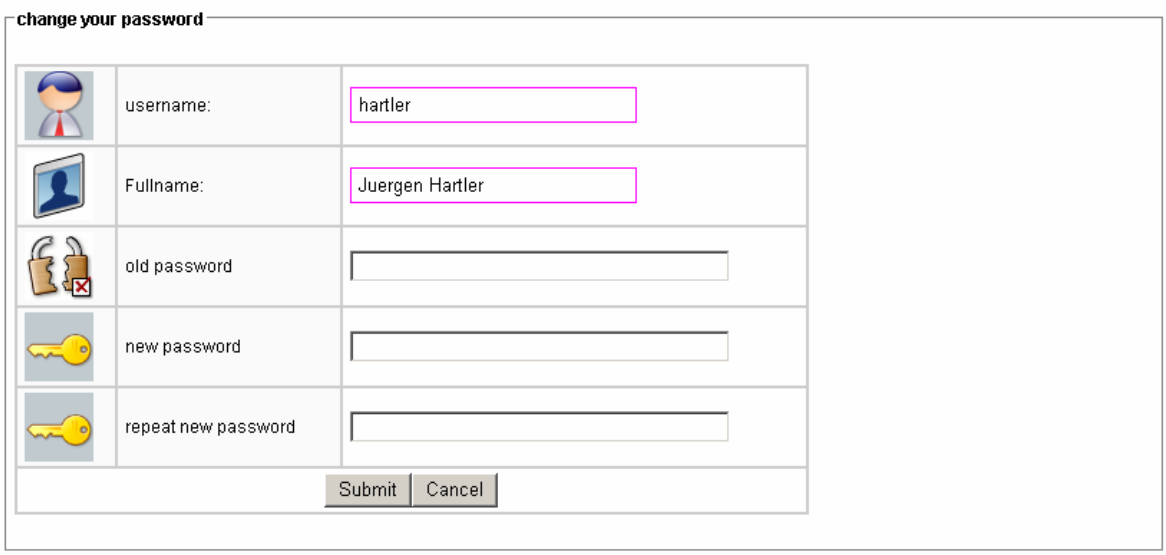
gives the possibility to log in

If you are logged in:

gives the possibility to:

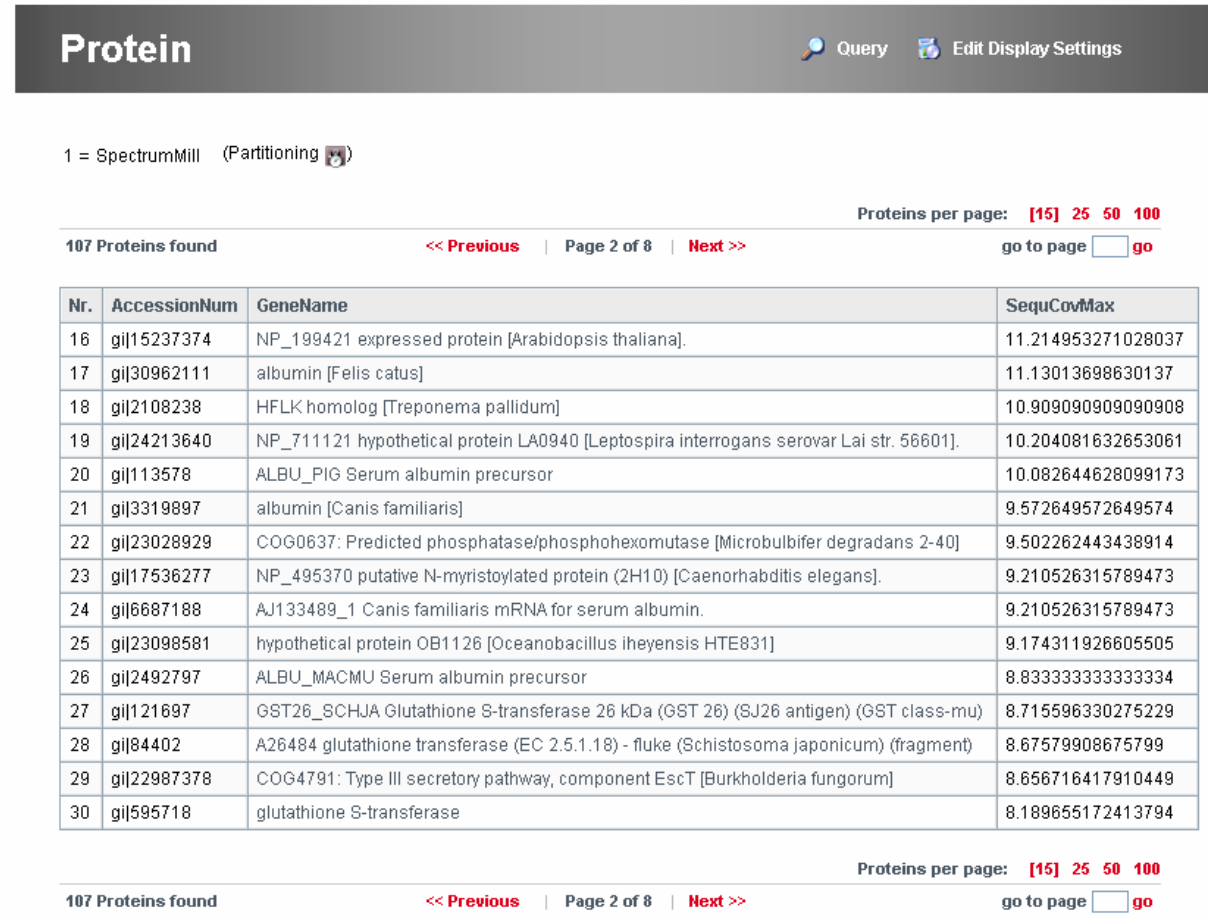
- Log out
- Show detailed information about your user account
- Change your password
- Displays your user

1.1.2.1 Change Password:



You must enter your old password and repeat the new one two times. The password must have at least 8 characters. One character must be a number and one character must be special character (!”@=?...).

1.2 The information section:



Nr.	AccessionNum	GeneName	SequCovMax
16	gi|15237374	NP_199421 expressed protein [Arabidopsis thaliana].	11.214953271028037
17	gi|30962111	albumin [Felis catus]	11.13013698630137
18	gi|2108238	HFLK homolog [Treponema pallidum]	10.909090909090908
19	gi|24213640	NP_711121 hypothetical protein LA0940 [Leptospira interrogans serovar Lai str. 56601].	10.204081632653061
20	gi|113578	ALBU_PIG Serum albumin precursor	10.082644628099173
21	gi|3319897	albumin [Canis familiaris]	9.572649572649574
22	gi|23028929	COG0637: Predicted phosphatase/phosphohexomutase [Microbulbifer degradans 2-40]	9.502262443438914
23	gi|17536277	NP_495370 putative N-myristoylated protein (2H10) [Caenorhabditis elegans].	9.210526315789473
24	gi|6687188	AJ133489_1 Canis familiaris mRNA for serum albumin.	9.210526315789473
25	gi|23098581	hypothetical protein OB1126 [Oceanobacillus iheyensis HTE831]	9.174311926605505
26	gi|2492797	ALBU_MACMU Serum albumin precursor	8.833333333333334
27	gi|121697	GST26_SCHJA Glutathione S-transferase 26 kDa (GST 26) (SJ26 antigen) (GST class-mu)	8.715596330275229
28	gi|84402	A26484 glutathione transferase (EC 2.5.1.18) - fluke (Schistosoma japonicum) (fragment)	8.67579908675799
29	gi|22987378	COG4791: Type III secretory pathway, component EscT [Burkholderia fungorum]	8.656716417910449
30	gi|595718	glutathione S-transferase	8.189655172413794

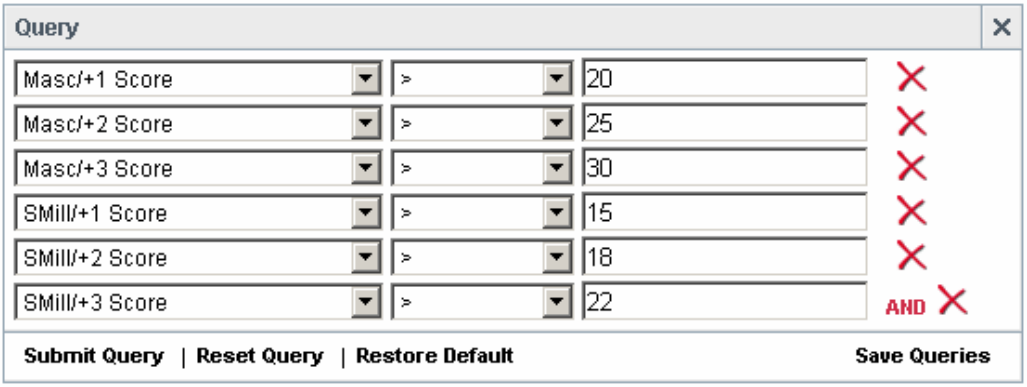
The general presentation of the data in MASPECTRAS looks like the figure above.
In the header section there are 2 links:

- Customizable queries
- Customizable display

The table with the data is always enclosed by the bars for the scrolling and almost every column in the table is sortable.

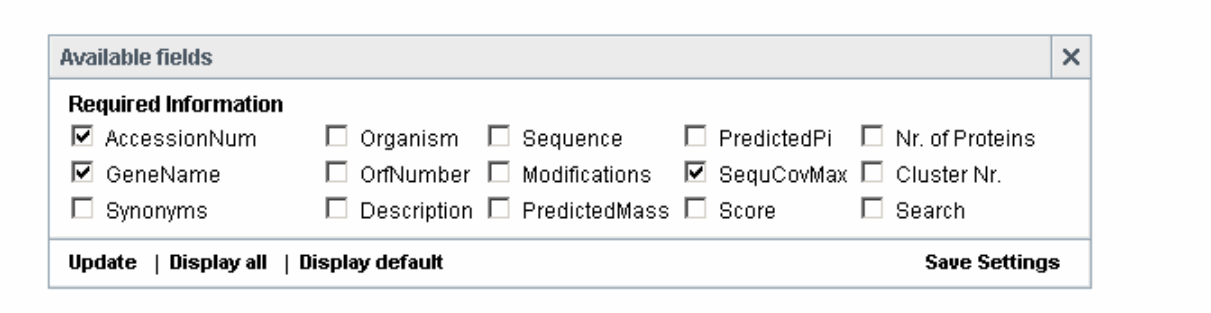
If you come from another page, at the bottom of the page, there is a return button, which brings you to page you have visited before.

1.2.1 Customizable queries:



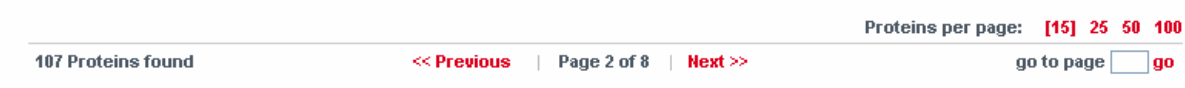
The query box enables the combination of as many queries as you like. The queries can be added or removed. The operators “LIKE” and “NOT LIKE” need a preceding or trailing asterisk
The button “Submit Query” submits the entered query and changes the view on the data correspondingly.
“Reset Query” removes all entered queries and submits a query without any user-defined filters.
Restore Default” restores the default set of queries and submits them.
“Save Queries” saves the actually entered set of queries as default to the database and submits them. Unless you change the queries your data on that page will always be filtered with this default set of queries.

1.2.2 Customizable display:



The information that will be displayed on the screen is customizable to the needs of the end-user. The user can select the information by clicking on the checkboxes and update the view on the data by pressing the button “Update”.
“Save Settings” allows the user to store his own display settings. Whenever the user enters the same page his settings will be displayed by default.

1.2.3 Scrolling bar:



On the left the scrolling bar shows the number of elements that have been found (depending on the query the user submitted). In the centre section the total number of pages with the actual page is displayed, plus the two arrows to go to next or the previous page. In the centre section the actual page is displayed and it is possible to switch to the previous and the next page. On the right you can choose how many proteins you prefer to be shown on one page. At the right side you can define the number of items per page and you jump to any page by entering the page number and pushing the "go" button.

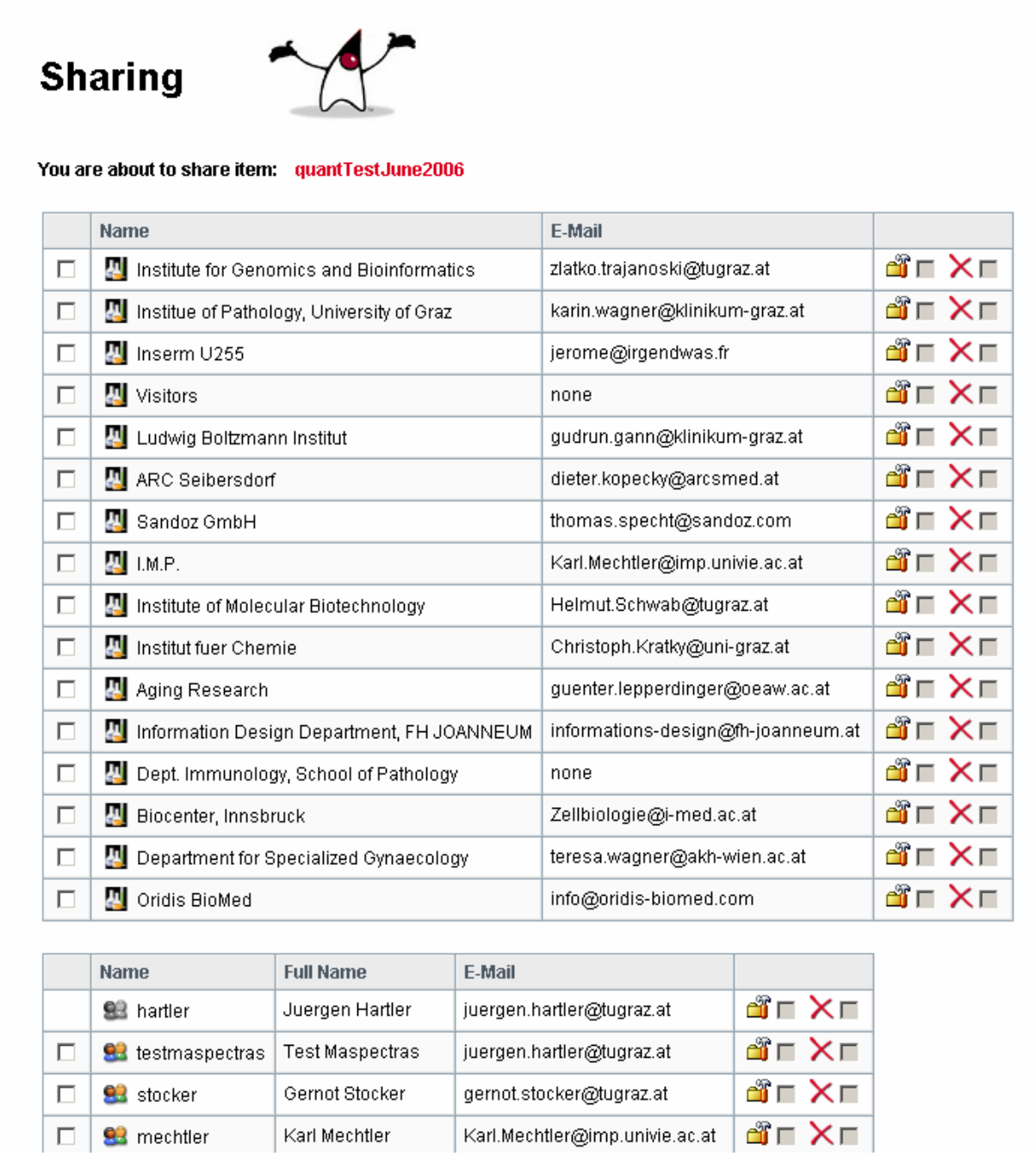
Nr.	ID	Upload Name	Category	Added Date				
1	2650	casein_NL_MS3	xcalibur	2005-06-29				
2	2700	Task1ms22400-3601	sequest	2005-07-06				
3	2600	testBigMascot	mascot	2005-06-21				
4	2850	newMascot	mascot	2005-08-04				
5	2001	karlDB	synthDatabase	2005-06-07				
6	2002	kPEP_phospho_BSA	synthDatabase	2005-06-07				
7	2003	myTestDB	synthDatabase	2005-06-07				
8	2004	SynthDB	synthDatabase	2005-06-07				
9	2005	SynthPep	synthDatabase	2005-06-07				
10	2006	SpectrumMill	spectrummill	2005-06-07				
11	2007	Task1ms22400-3600	sequest	2005-06-07				
12	2009	Task2synthDBAll	sequest	2005-06-07				
13	2010	Task2testKarlDB2	sequest	2005-06-07				
14	2011	Task2CompToMasc	sequest	2005-06-07				
15	2012	MSDB	mascot	2005-06-07				

The table view consists by default of the following parts:

- The header: if you hover your mouse over a column-name the colour changes to blue and you can sort by this column
- The number in the first column indicates the hit number of the entry corresponding to the order you sorted your data
- Links to data connected to the entries are normally located on entries in the list
- : Indicates that you can edit your data here.
- : Indicates if there is some information downloadable

- : Indicates if you can delete this data entry here.
- : Indicates that there is additional information available
- : Indicates that you can share your data to other users of the system

When you click on the share icon you move to a page where you can select other users or institutes and make the data available for them:

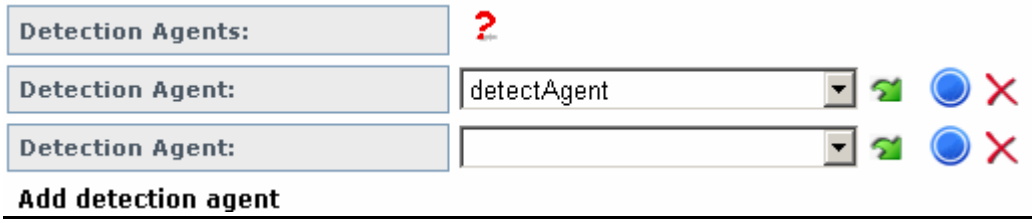


When you select a user or an institute the checkboxes at and are enabled and you can additionally specify if the user has edit or delete rights on your data.

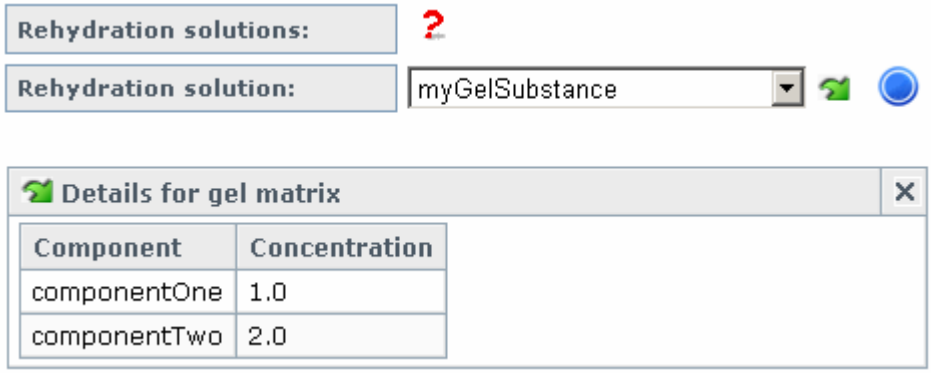
1.2.4 Select input Fields:

When you have an input field like the one above and your element of choice is not in the drop down menu, you can push the blue button and enter your element. The button can lead either to an input page of an element or to add dictionary elements. Dictionary elements are unified text elements. The main purpose is to overcome words with different spellings (or different level of detail in description) but the same meaning. For more detailed information about Dictionaries, see chapter 2.5 “Dictionary”.

1.2.5 Multiple input Fields and other buttons:

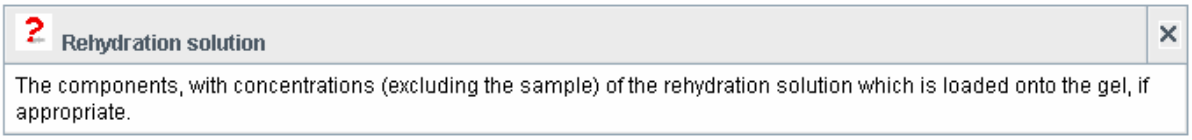


In MASPECTRAS there are very often multiple select or other input fields provided. With the “Add …” you can add additional input fields to your input mask, or with the you can remove them again. On **important** thing is, that when you add an object, or you any other changes, the changes will be stored in the database when you press the Update Button, while when you press the Button the data object will be deleted in the database, immediately.
When you press the Button you retrieve additional information about the selected object.



In this example the solution consists of two components and they are shown below the select field. When such a details field is open and you change the selected selection this field is updated automatically. Such fields can be closed again with the . When the button is next to an image the image is displayed at the bottom of the page.

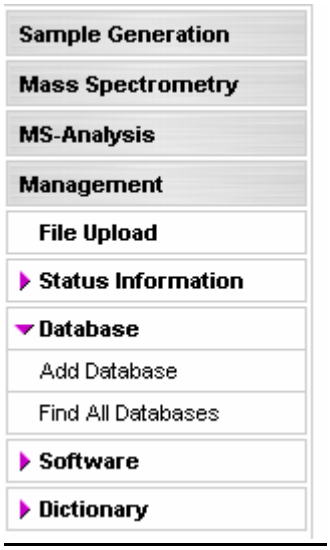
The provides you a help, so that it is clear what has to be entered at this input field. The information appears at the top of the page.



2. Management Section:

2.1 Database:

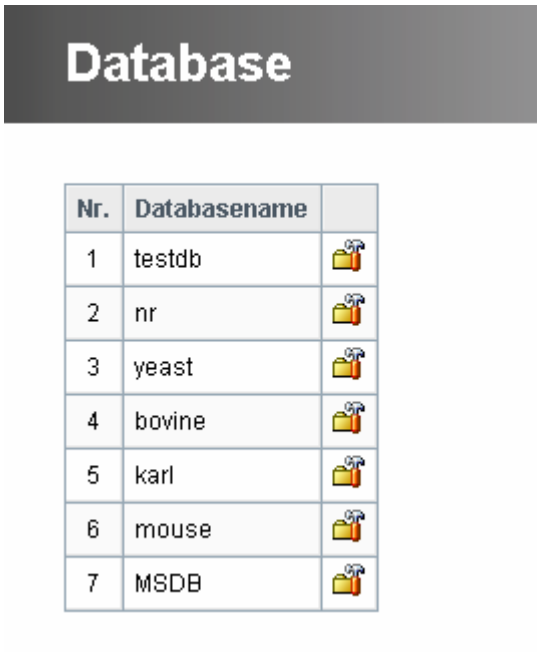
By clicking Management-> Database in the menu-bar you reach the general Database Section. MASPECTRAS needs the original sequence databases to find out the corresponding protein sequence.



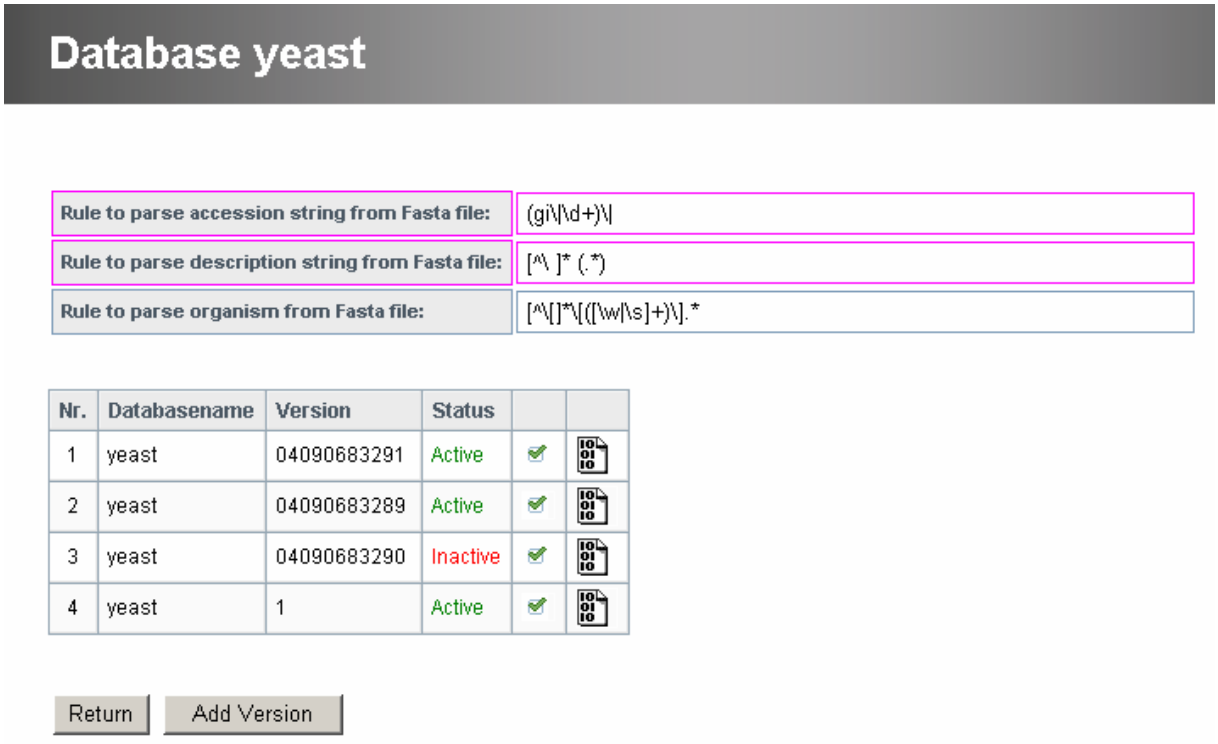
With the “Add Database” you can add a new database.

When you select a file, the fields databasename and version are filled out automatically. When you enter no version the version is set to 1 automatically.

With the “Find All Databases” you get an overview of all your databases.



When you have created a database or pushed the button you get to the detailed view of your database:



At the top you can define your parsing rules for the accession string, the description string and the organism string. The accession rule and the description rule are mandatory. With the green checkbox you can test your parsing rules and you get the output of the first 10 entries at the bottom of this page:

```
================================================================
Complete Entry:
>gi|19114688|ref|NP_593776.1| hypothetical homeobox domain protein [Schizosaccharomyces pombe]□gi|1723488|sp|Q103
MRSYSNPENGGQINDNINYSEKRPTMLPENLSLSNYDMDSFLGQFPSDNNMQLPHSTYEQHLQGEQQNPTNPNYFPPEFD
ENKVDWKQEKPKPDAPSFADNNSFDNVNSSKLTNPSPVQPNIVKSESEPANSKQNEVVEATSVEKAKENVAHESGTPESG
GSTSAPKSKKQRLTADQLAYLLREFSKDTNPPPAIREKIGRELNIPERSVTIWFQNRRAKSKLISRRQEEERQRILREQR
ELDSLNQKVSQAFAHEVLSTSPTSPYVGGIAANRQYANTLLPKPTRKTGNFYMKSGPMQSSMEPCIAESDIPIRQSLSST
YYNSLSPNAVPVSSQRKYSASSYSAIPNAMSVSNQAFDVESPPSSYATPLTGIRMPQPESDLYSYPREVSPSSGGYRMFG
HSKPSSYKASGPVRPPNMATGHMRTSSEPTSYDSEFYYFSCTLLVIGLWKRLRASPQDLMCFYSPPKKLFAYLIQFQGIQ
YRIEYSFFVIESIHVFRVEEPLLNELSATASSRDKPAPNEYWLQMDIQLSVPPVFHMITSEGQGNCTDFTEGNQASEVLL
HSLMGRATSMFQMLDRVRRASPELGSVIRLQKGLNPHQFLDPQWANQLPRQPDSSVFDHQGRNPPIQGLSHDTSSEYGNK
SQFKRLRSTSTPARQDLAQHLLPPKTNTEGLMHAQSVSPITQAMKSANVLEGSSTRLNSYEPSVSSAYPHHNLALNLDNT
QFGELGTSNISYPLSAPSDVGSLPRASNSPSRPVMHPNTQGINTEIKDMAAQFPNSQTGGLTPNSWSMNTNVSVPFTTQN
REFGGIGSSSISTTMNAPSQQLSQVPFGDVSLATENSVPSYGFEVPSEESVYAQARTNSSVSAGVAPRLFIQTPSIPLAS
SAGQDSNLIEKSSSGGVYASQPGASGYLSHDQSGSPFEDVYSPSAGIDFQKLRGQQFSPDMQ

Rule accession_rule: gi|19114688,gi|1723488,gi|7490714,gi|1213267,
Rule description_rule: hypothetical homeobox domain protein [Schizosaccharomyces pombe],Hypothetical protein C32A
Rule organism_rule: Schizosaccharomyces pombe,null,null,Schizosaccharomyces pombe,
================================================================
Complete Entry:
>gi|496693|emb|CAA56020.1| B-127 protein [Saccharomyces cerevisiae]
MPFSFLAQPFPPCKISSTHSLGVNSPGRGSHGNLNVFWYKLSISGLIEEDIVVDSPGFVVISLLLWLVEVGDLILVLFPV
AFVPGFATVVPIPLKLENVFLGDIWFVVDVGLDSSDVLSSIVFIPGL

Rule accession_rule: gi|496693
Rule description_rule: B-127 protein [Saccharomyces cerevisiae]
Rule organism_rule: Saccharomyces cerevisiae
================================================================
Complete Entry:
>gi|6323056|ref|NP_013128.1| AICAR transformylase/IMP cyclohydrolase; Ade16p [Saccharomyces cerevisiae]□gi|170991
MGKYTKTAILSVYDKTGLLDLAKGLVENNVRILASGGTANMVREAGFPVDDVSSITHAPEMLGGRVKTLHPAVHAGILAR
NLEGDEKDLKEQHIDKVDFVVCNLYPFKETVAKIGVTVQEAVEEIDIGGVTLLRAAAKNHSRVTILSDPNDYSIFLQDLS
KDGEISQDLRNRFALKAFEHTADYDAAISDFFRKQYSEGKAQLPLRYGCNPHQRPAQAYITQQEELPFKVLCGTPGYINL
LDALNSWPLVKELSASLNLPAAASFKHVSPAGAAVGLPLSDVERQVYFVNDMEDLSPLACAYARARGADRMSSFGDFIAL
SNIVDVATAKIISKEVSDGVIAPGYEPEALNILSKKKNGKYCILQIDPNYVPGQMESREVFGVTLQQKRNDAIINQSTFK
EIVSKNKALTEQAVIDLTVATLVLKYTQSNSVCYAKNGMVVGLGAGQQSRIHCTRLAGDKTDNWWLRQHPKVLNMKWAKG
IKRADKSNAIDLFVTGQRIEGPEKVDYESKFEEVPEPFTKEERLEWLSKLNNVSLSSDAFFPFPDNVYRAVQSGVKFITA
PSGSVMDKVVFQAADSFDIVYVENPIRLFHH

Rule accession_rule: gi|6323056,gi|1709914,gi|7433574,gi|1480728,gi|2204263,
Rule description_rule: AICAR transformylase/IMP cyclohydrolase; Ade16p [Saccharomyces cerevisiae],Bifunctional pu
Rule organism_rule: Saccharomyces cerevisiae,null,null,null,Saccharomyces cerevisiae,
================================================================
```

First you get the complete database entry. At “Rule accession_rule:” you get your returned accession strings. If there are multiple ones for one entry they are always separated by “,”. It is mandatory that the accession string that you see here is the same like in your result files because this one is used for the indexing. At “Rule description_rule” you get the description of your protein. At “Rule organism_rule:” you get the result of your organism rule. If there is a “null” within the string, than this rule didn’t return anything (happens sometimes, when there are no organisms declared). When you are content with your result push the  button to index your database. Examples for parsing rules you will find in your installation package at /doc/parsingRules

The database can have the following stati:

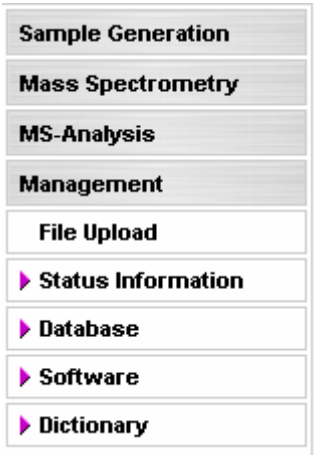
Active : The database is active and can be used for file parsing.

Indexing : This database is indexing. (This page is not refreshed automatically at the moment)

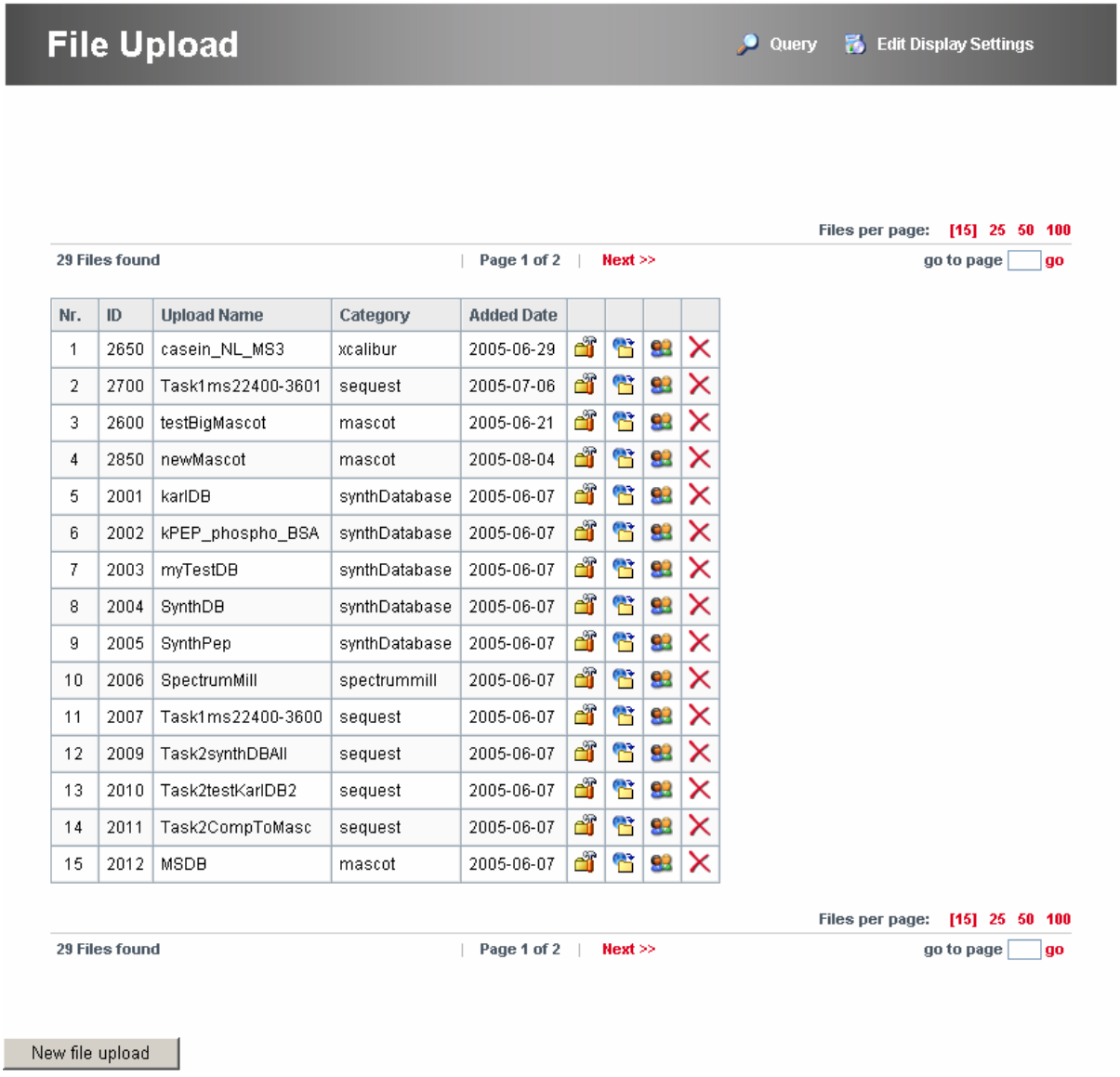
Inactive : The database has not been indexed or something at the indexing has gone wrong

It is not mandatory to keep all the versions of your databases. Once a search result file has been parsed into MASPECTRAS it stays conserved and does not need the old database again. The database section should be reserved to an administrator of MASPECTRAS, because when the definition string is changed in a running instance, you have to be aware that there may be pending data uploads which need information with the old settings. Once the data is uploaded into MASPECTRAS there is no need to keep the old database, the whole sequence is stored within MASPECTRAS.

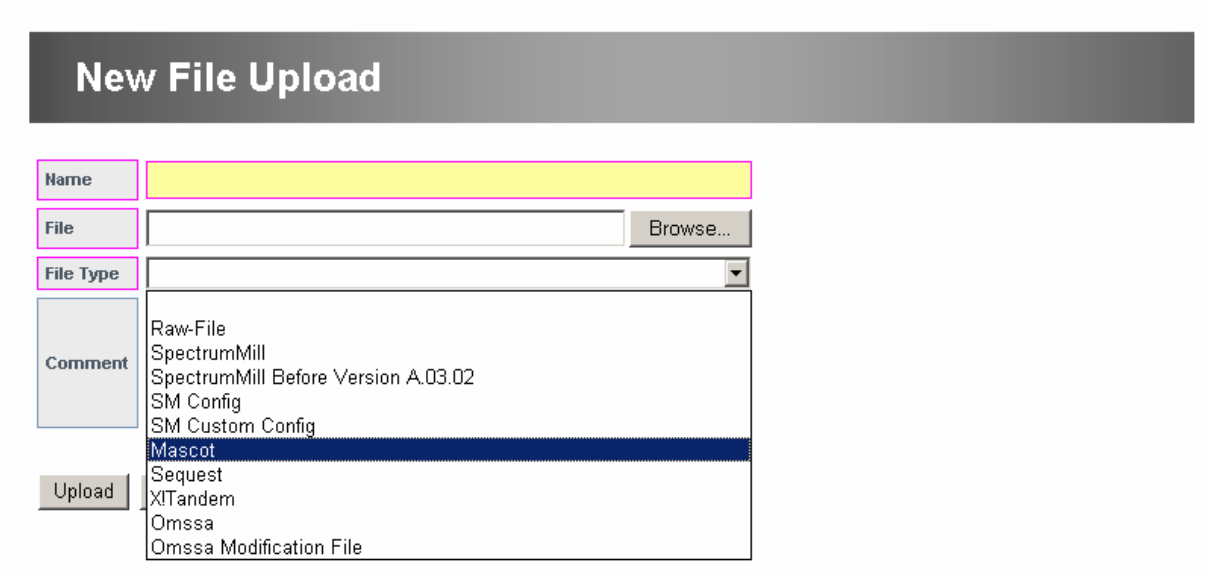
2.2 File Upload:



By clicking Management->FileUpload in the menu-bar you reach the general Upload Section, where all your already uploaded files are listed:



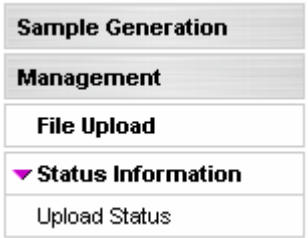
With “New file upload” you come to the upload page:



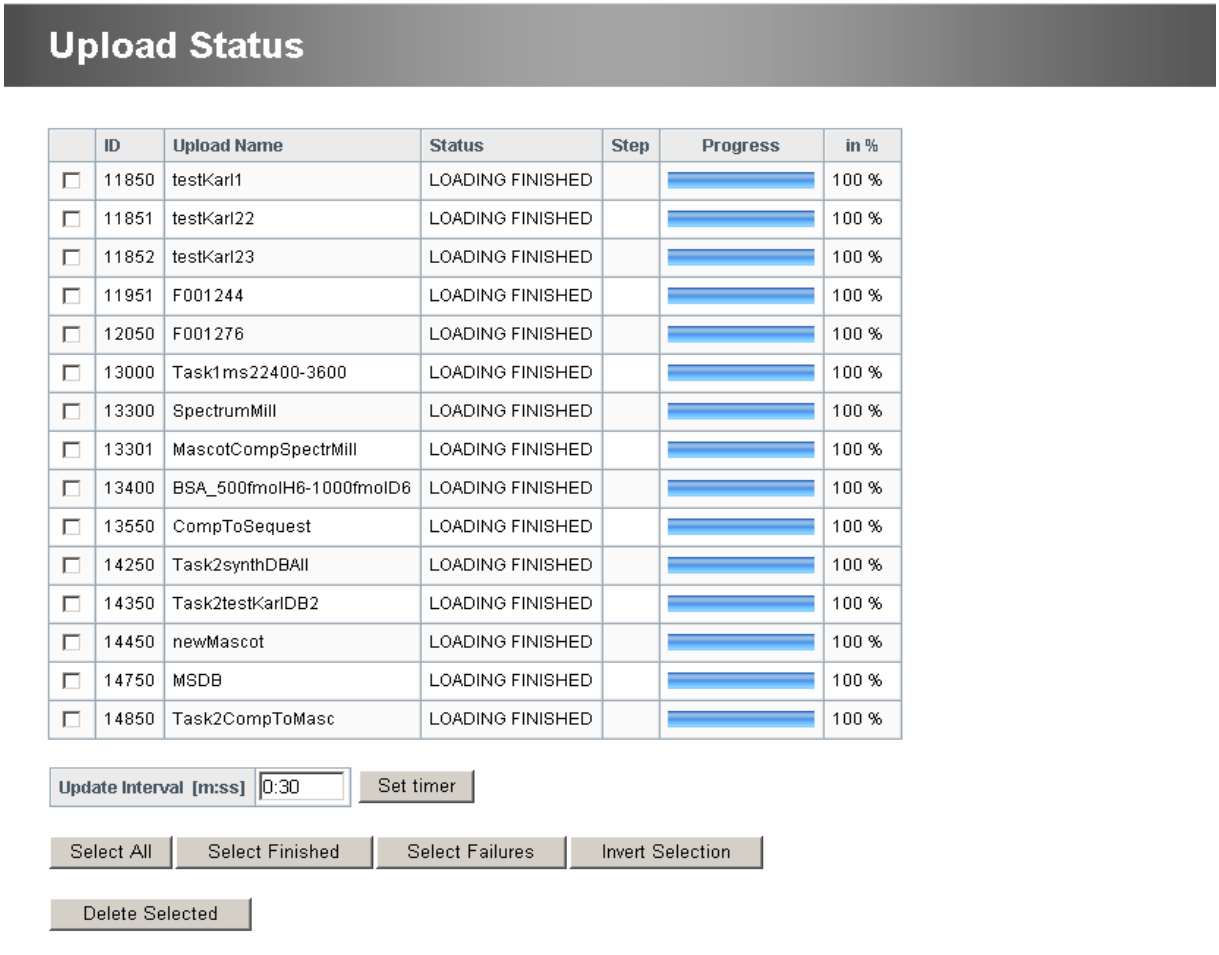
The important thing is that you have to add your file to the corresponding category.
The Sequest-Files and SpectrumMill-Files must be uploaded in a *.zip directory. Spectrum Mill is differentiated in “Spectrum Mill” (new version) and “Spectrum Mill Before Version A.03.02” (old version). For the new version a SM Config File (your smconfig.xml file) is necessary. The SM Custom Config (your smconfig.custom.xml) is not mandatory, but needed when you searched with modifications and elements which you created by yourself. For OMSSA searches the Omssa Modification File (mods.xml) is needed. As “Raw-File” mzXML, mzData and XCalibur Version 1.3 RAW are accepted.

2.3 Upload Status:

By clicking Management->Status Information->Upload Status in the menu-bar you reach the general Upload Status Section.

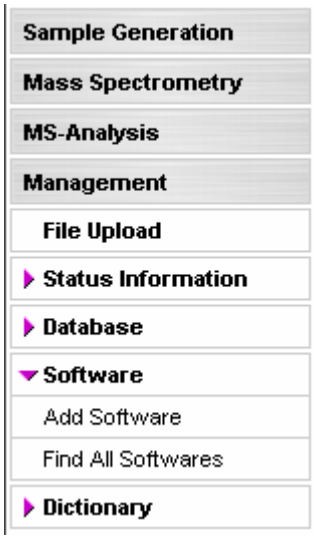


This page gives information about the progress of tasks, which are processed asynchronously because of their time consume.



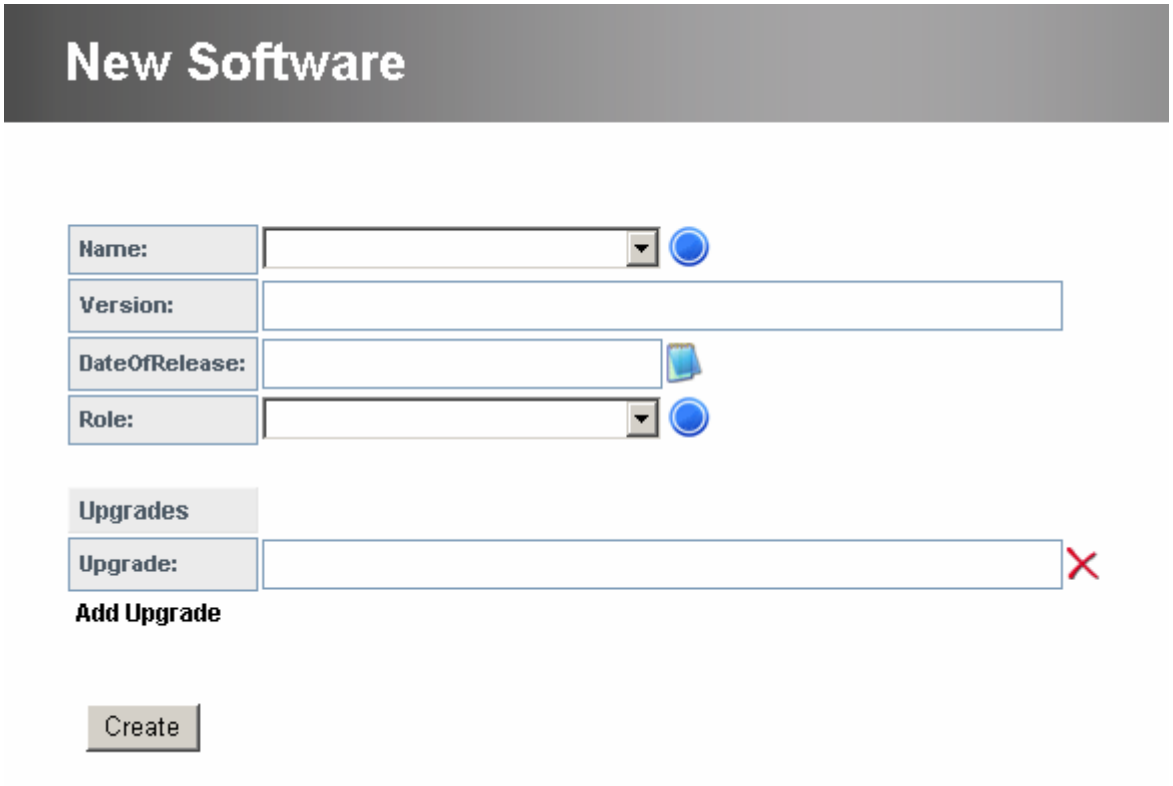
2.4 Software:

By clicking Management->Software in the menu-bar you reach the general Software Section.



The general software section is used to document all the software used in MASPECTRAS. Here you can get an overview about the software and edit them. When the software is needed in a select box in another table you can add new software from there directly (e.g. see chapter 5.5 “Controlsoftware”).

With “Add Software” you can add new software.

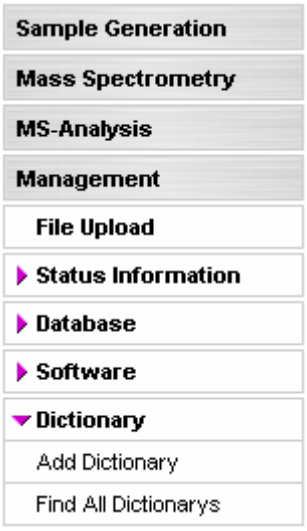


With the link “Add Upgrade” you can enter software upgrades.

With “Find All Softwares” you get an overview of all your general software.

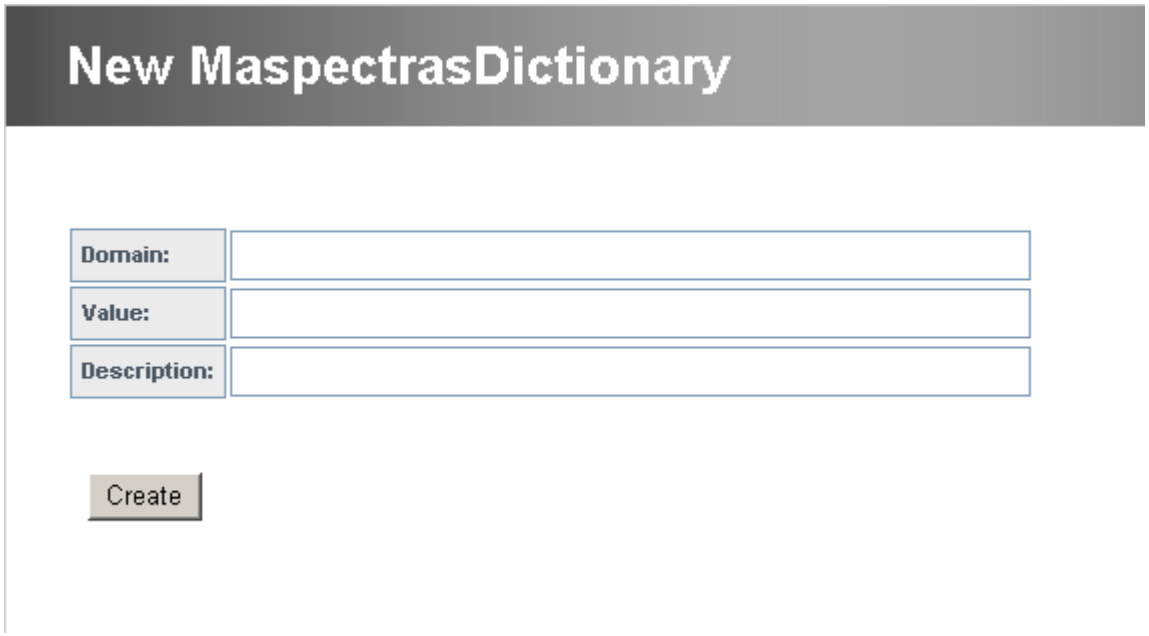
2.5 Dictionary:

By clicking Management->Dictionary in the menu-bar you reach the general dictionary section.

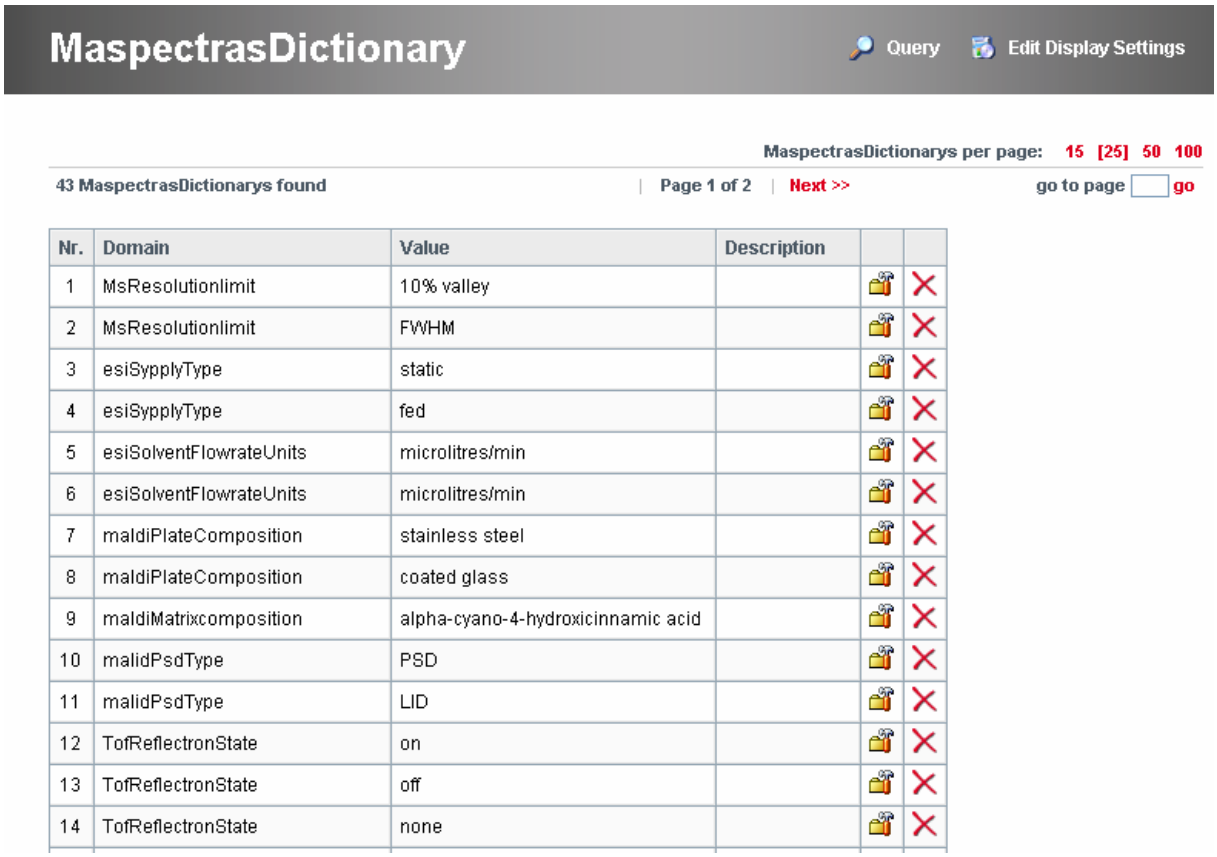


The dictionary section stores commonly used values for certain input fields. Here are you can add, edit and change dictionary values from all domains, while when you are in another table you can only select an existing dictionary field and add values for this certain domain.

With the “Add Dictionary” you can add a new dictionary entry.



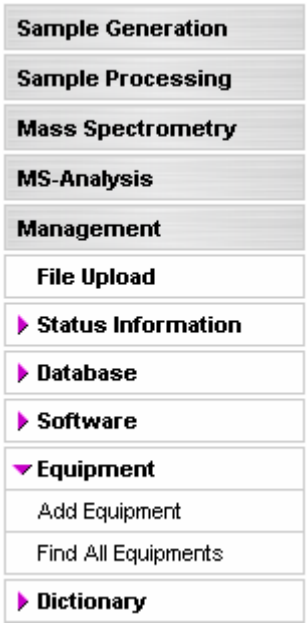
By clicking the “Find All Dictionarys” you will get an overview of all your dictionaries.



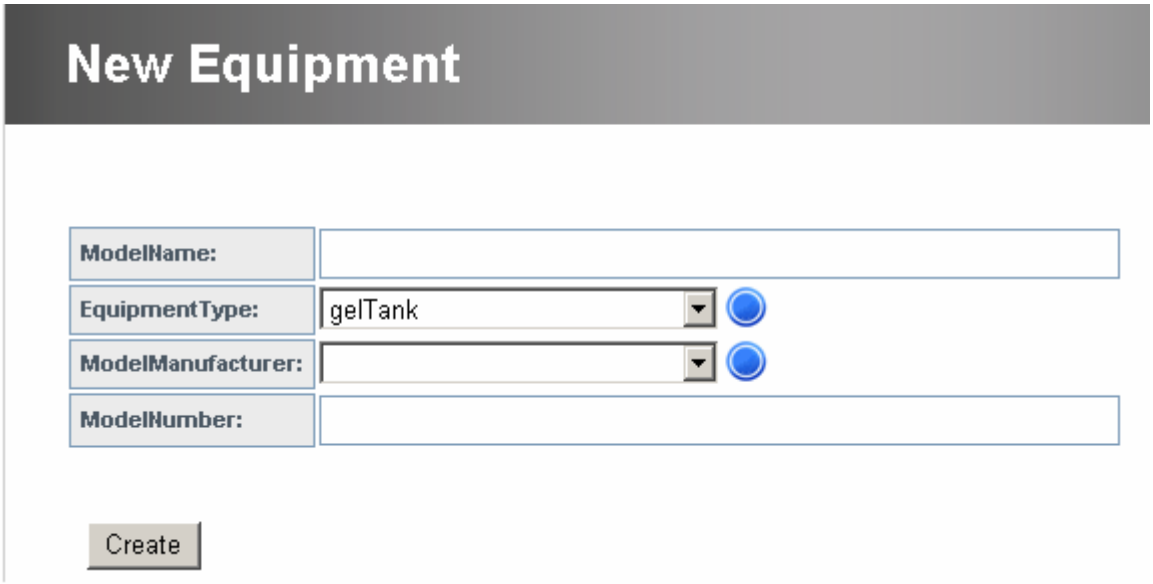
Nr.	Domain	Value	Description		
1	MsResolutionlimit	10% valley			
2	MsResolutionlimit	FWHM			
3	esiSypplyType	static			
4	esiSypplyType	fed			
5	esiSolventFlowrateUnits	microlitres/min			
6	esiSolventFlowrateUnits	microlitres/min			
7	maldiPlateComposition	stainless steel			
8	maldiPlateComposition	coated glass			
9	maldiMatrixcomposition	alpha-cyano-4-hydroxicinnamic acid			
10	malidPsdType	PSD			
11	malidPsdType	LID			
12	TofReflectronState	on			
13	TofReflectronState	off			
14	TofReflectronState	none			

2.6 Equipment:

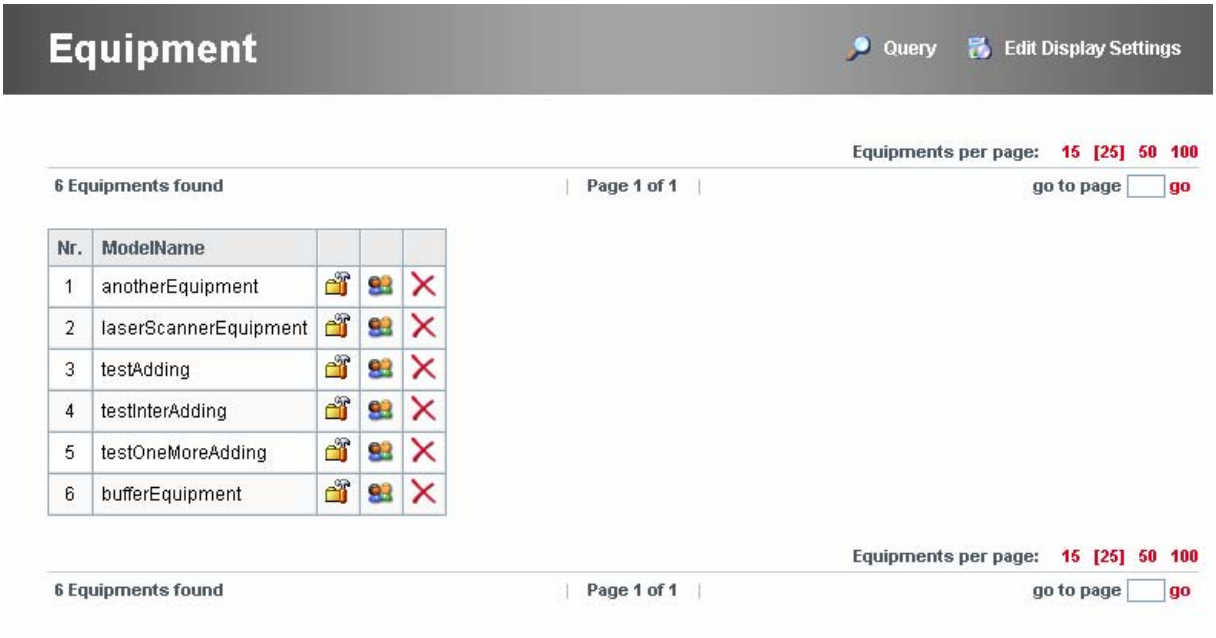
By clicking Management->Equipment in the menu-bar you reach the general equipment section.



The equipment section stores all kinds of equipment needed (for 1D Gels, 2D Gels, …). With the “Add Equipment” you can add a new equipment entry.



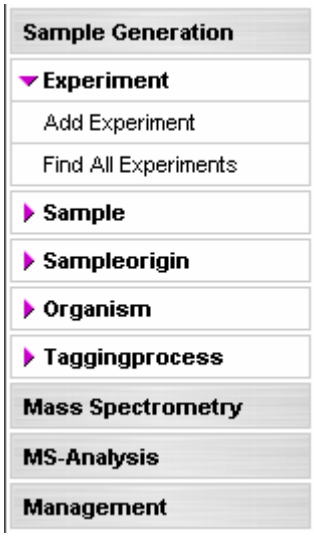
Because of the fact that the equipment section is general, it is necessary to enter the type of the equipment. Then it is easier to find the wanted one.
By clicking the “Find All Equipments” you will get an overview of all your dictionaries.



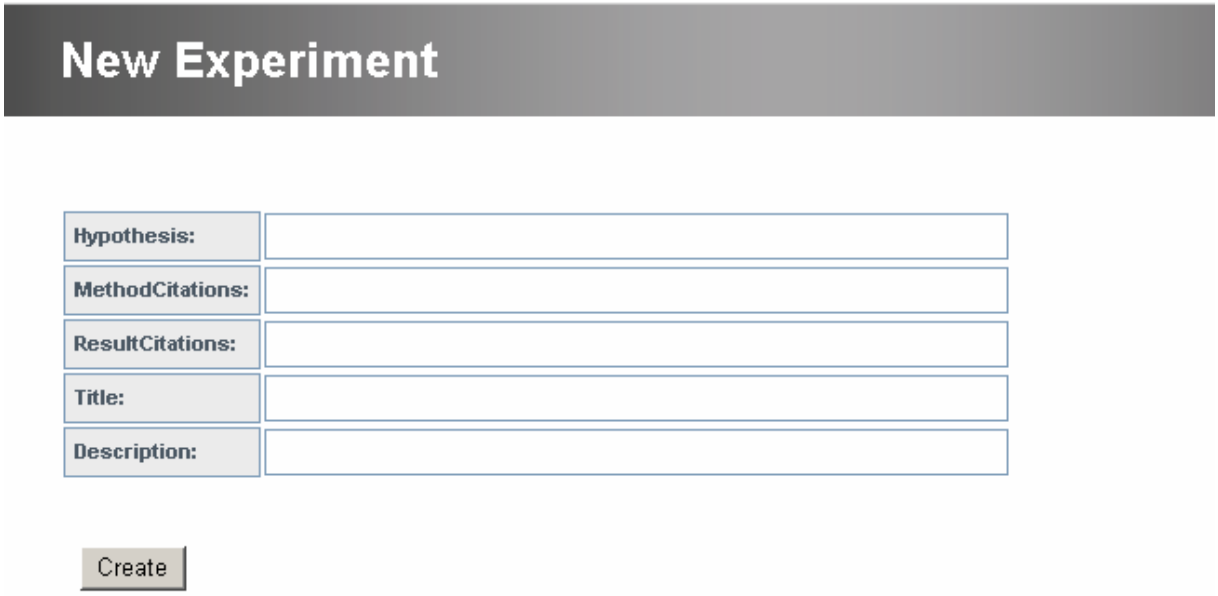
3. Sample Description:

3.1 Experiment:

By clicking Sample Generation->Experiment you reach the experiment section.



With the “Add Experiment” you can add new experiments.



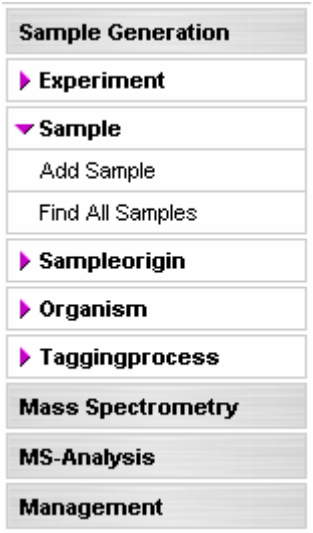
With the “Find All Experiments” you get an overview of all your experiments.

3.2 Sample:

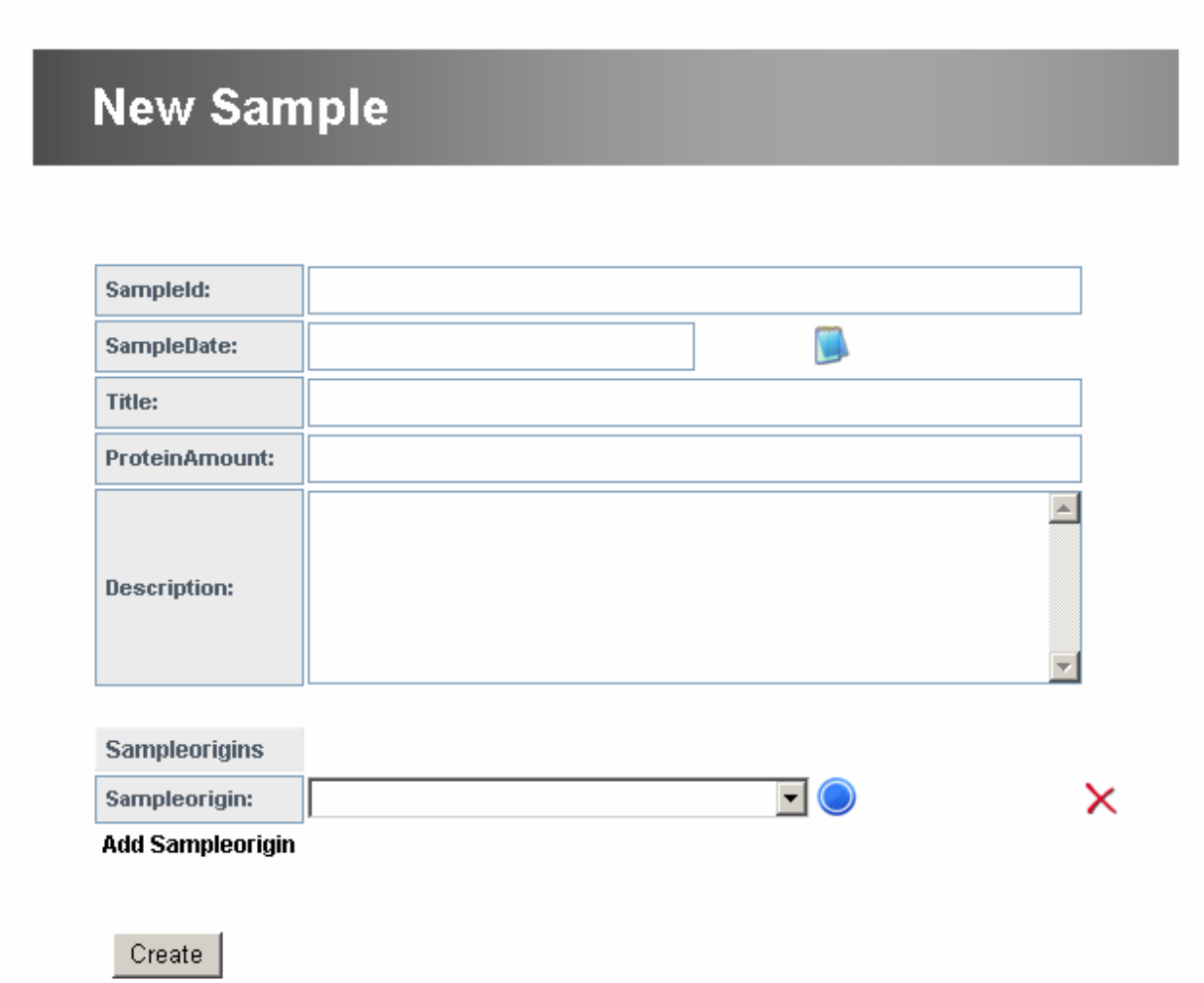
There are 2 ways to generate your sample:

3.2.1 Sample directly:

Here it works in the same way like in the experiment.
By clicking Sample Generation->Sample you reach the sample section.

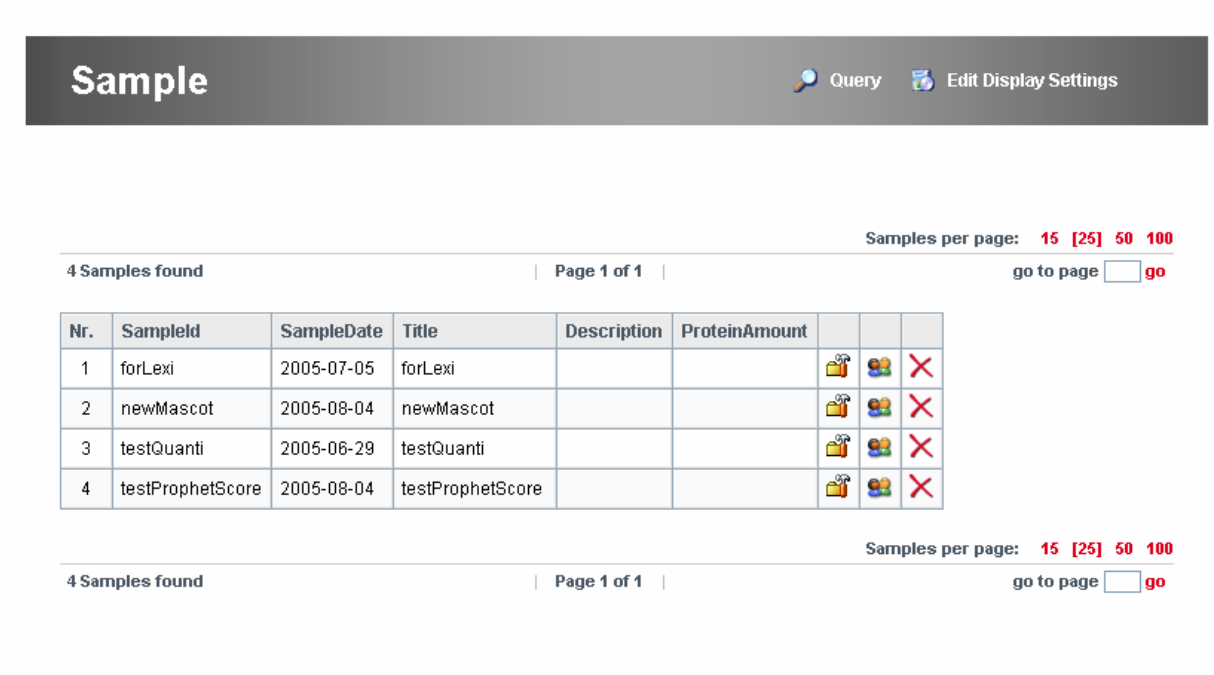


With the “Add Sample” you can add a new sample:



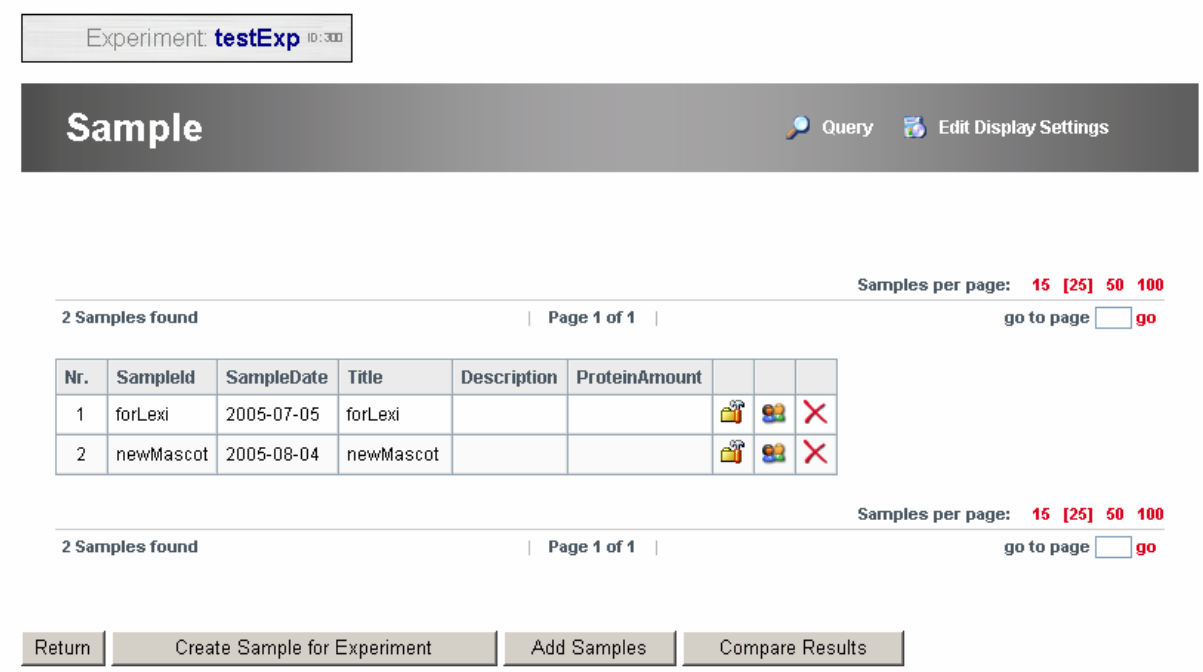
With the link on “Add Sampleorigin” you can add additional origins to the sample. If your desired sample origin is not in the list you can add it directly with the blue button on the right side of the select field. Read more about sample origins in chapter 3.3 “Sampleorgin”.

With a click on the button “Find All Samples” you get an overview of all your samples:



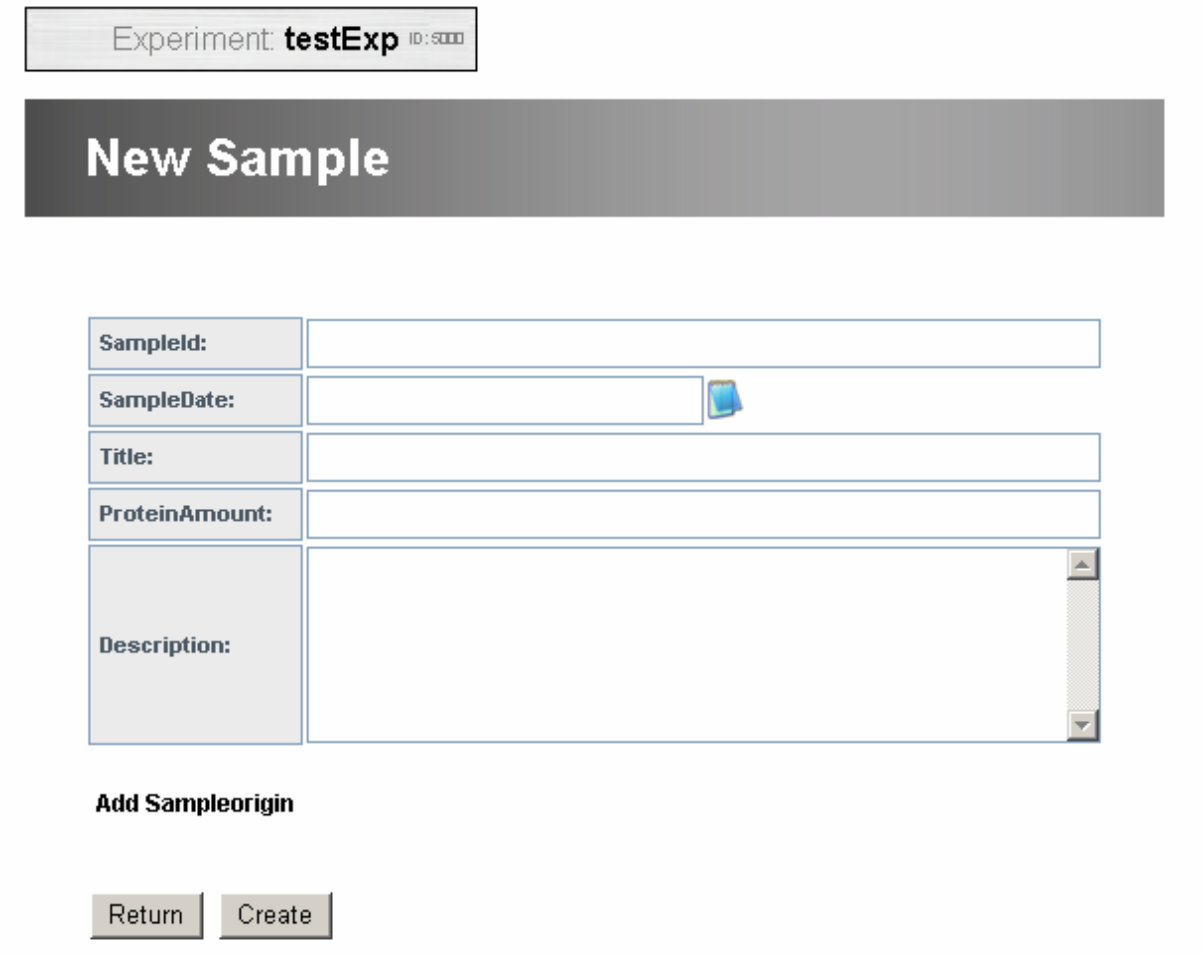
3.2.2 Sample over experiment:

When you click on the title of your experiment where you are interested in then you get an overview of all your samples which has been added to this experiment.

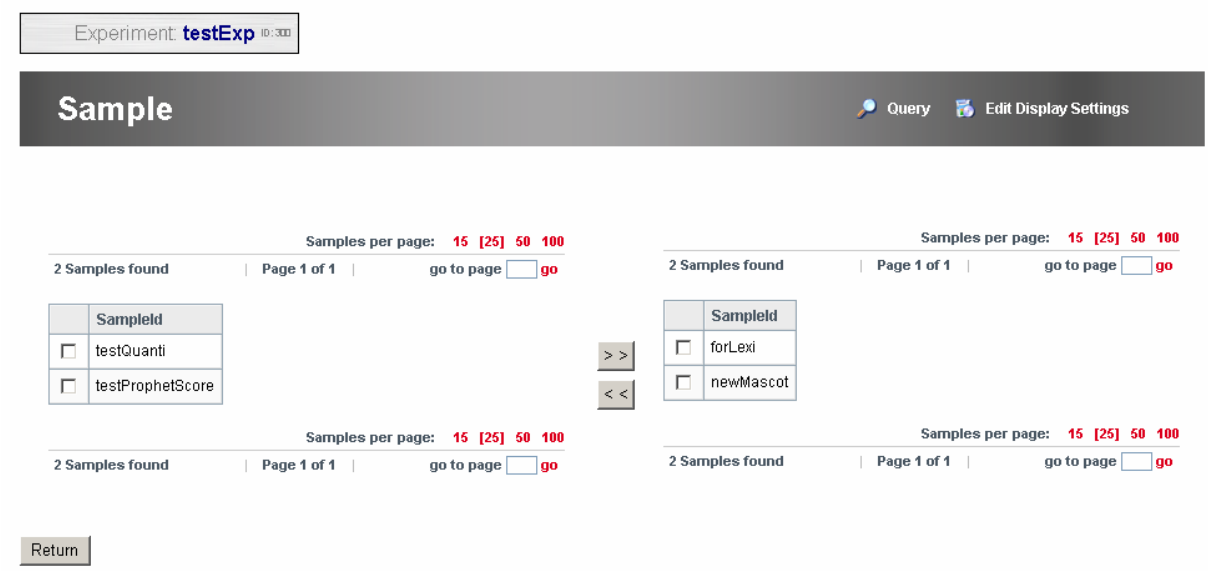


With the link at the top of the page (in this case “testExp”) you will get back to this page when you are in a lower level of the program.

When you push the “Create Sample for Experiment” button you can generate a new sample and it will be added directly to the experiment.



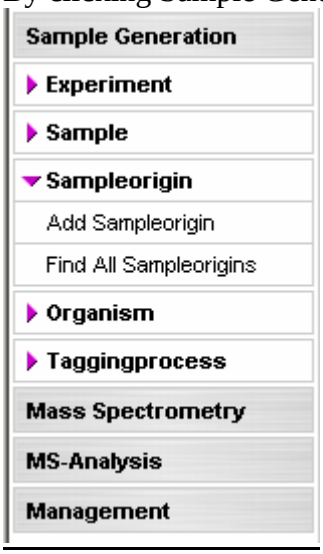
When you use the “Add Samples” button you can add or remove existing samples to or from your experiment.



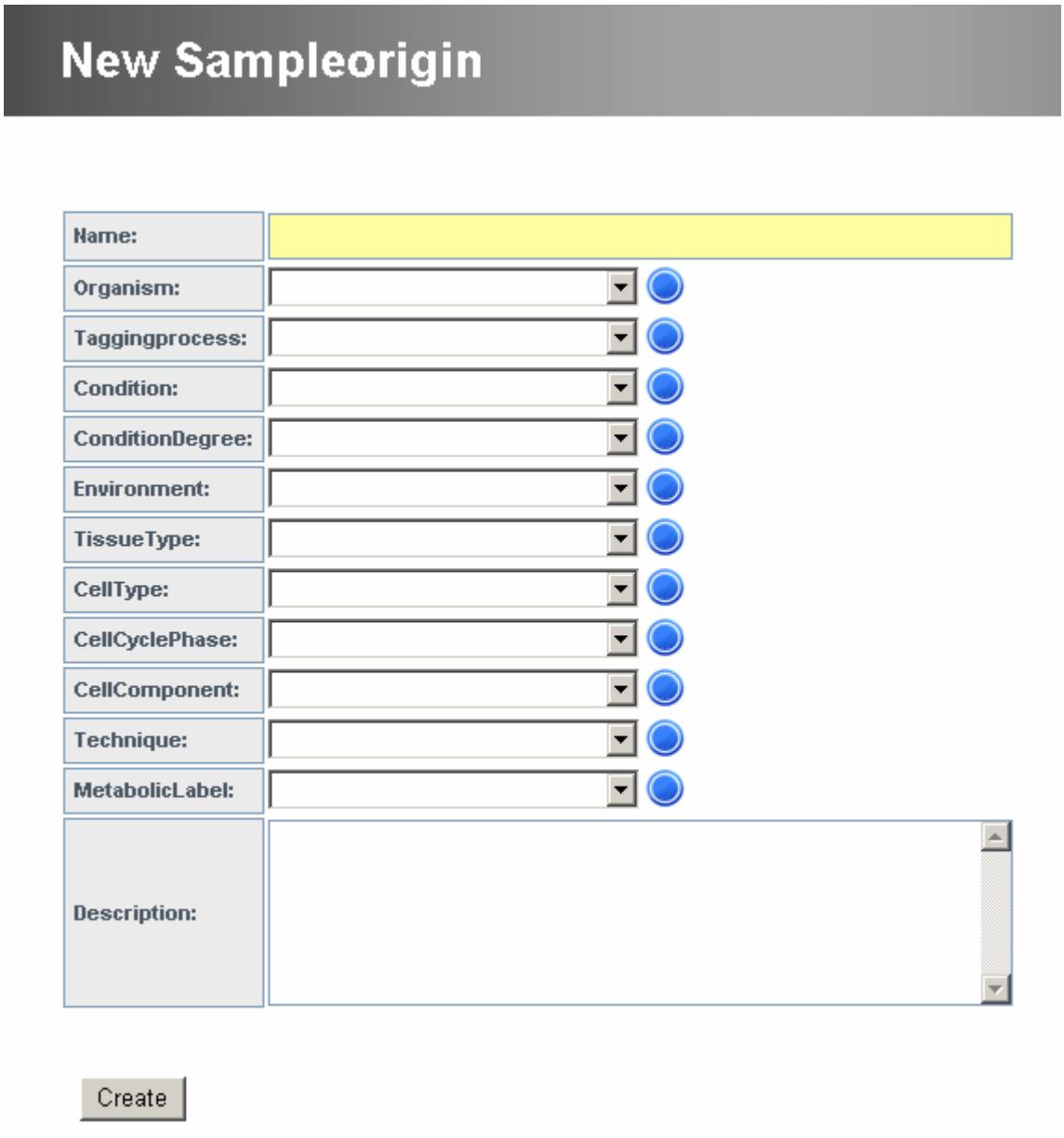
On the left side the addable samples are listed and on the right side the already added samples are listed. The left side is completely queryable. When you want to add samples you simply check the desired checkboxes of the samples on the left side and push the “>>” button. When you want to remove samples you simply check the desired checkboxes of the samples on the right side and push the “<<” button.
The meaning of the “Compare Results” button will be explained in the Analysis section (4).

3.3 Sampleorigin:

By clicking Sample Generation->Sampleorgin you reach the sample origin section.

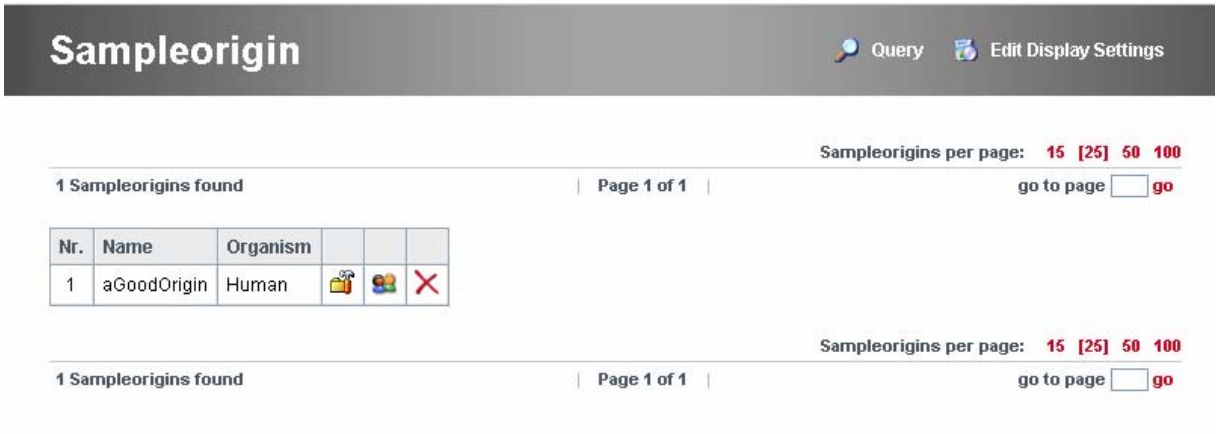


With the “Add Samplorigin” you can add new sample origins.



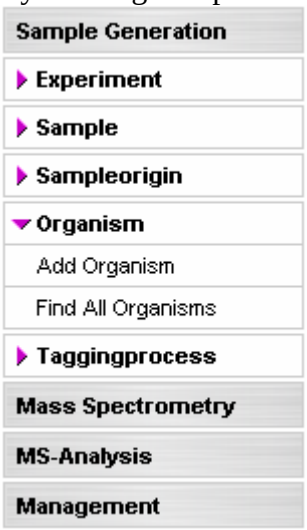
If your desired organism or tagging process is not in the list you can add it directly with the blue button on the right side of the select field. Read more about organisms in chapter 3.4 “Organism” and about tagging processes in chapter 3.5 “Taggingprocess”.

With a click on the button “Find All Sampleorigins” you get an overview of all your sample origins:

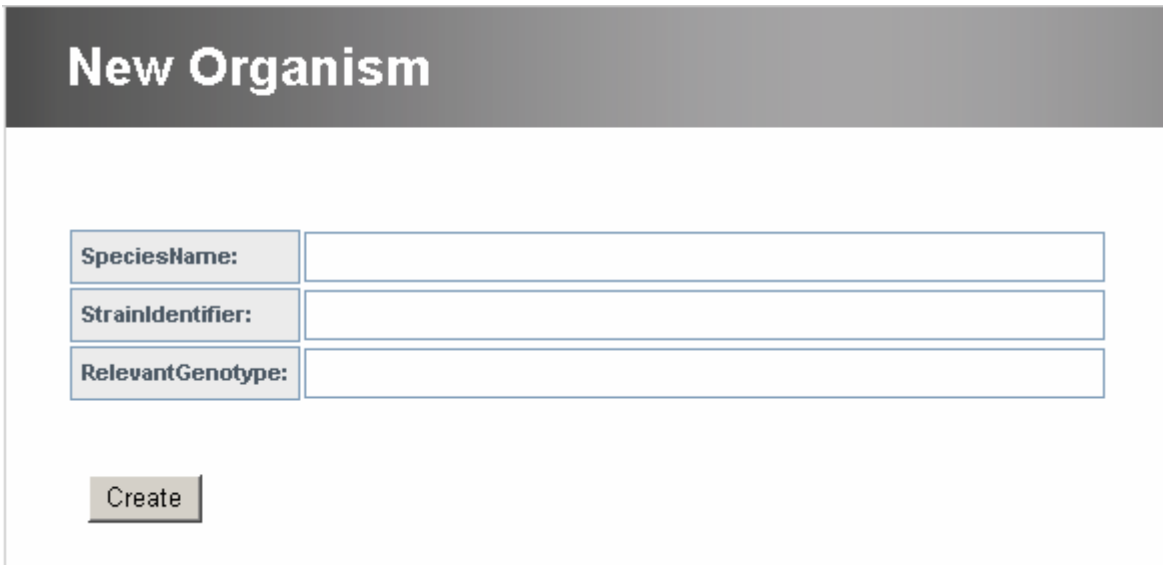


3.4 Organism:

By clicking Sample Generation->Organism you reach organism section.



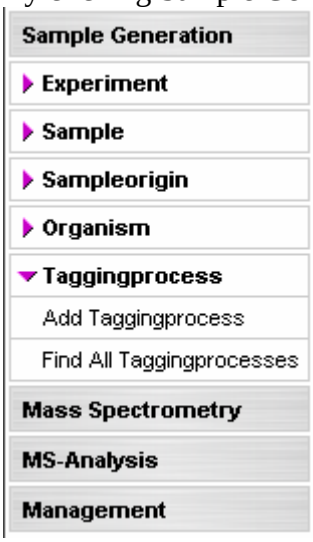
With the “Add Organism” you can add new organisms.



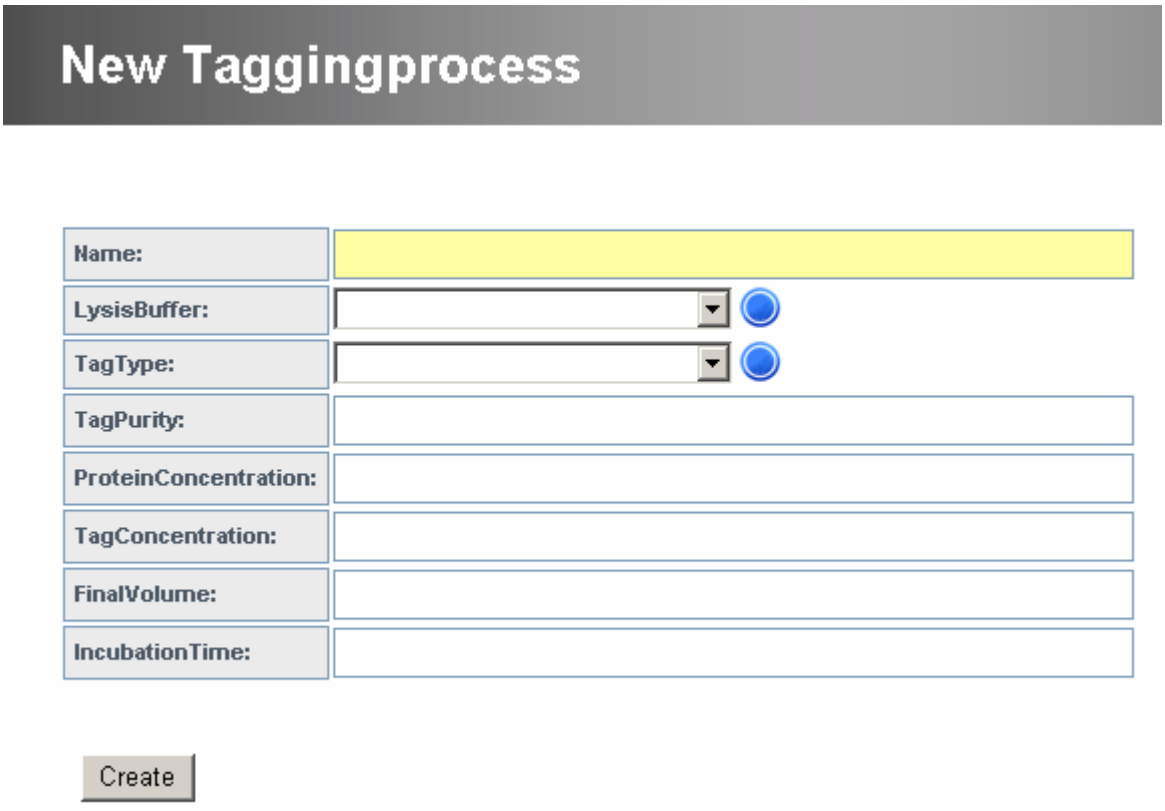
With a click on the button “Find All Organisms” you get an overview of all your organisms:

3.5 Taggingprocess:

By clicking Sample Generation->Taggingprocess you reach tagging process section.



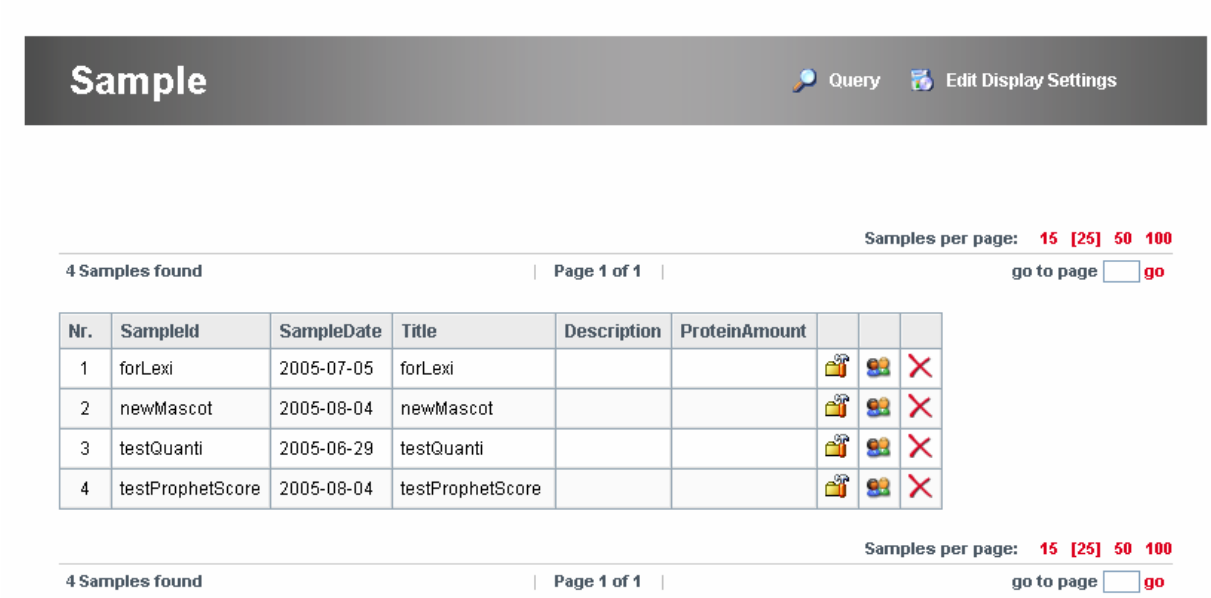
With the “Add Taggingprocess” you can add new tagging process.



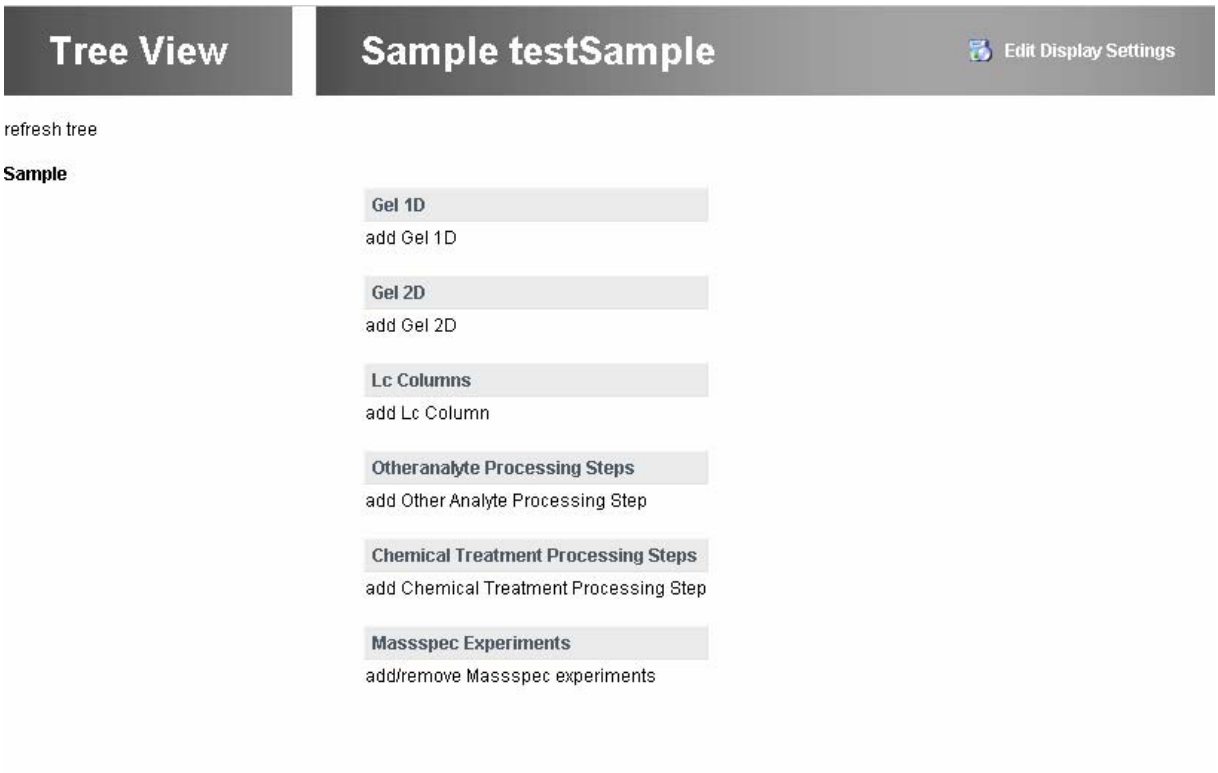
With a click on the button “Find All Taggingprocesses“ you get an overview of all your tagging processes:

4. Sample Preprocessing:

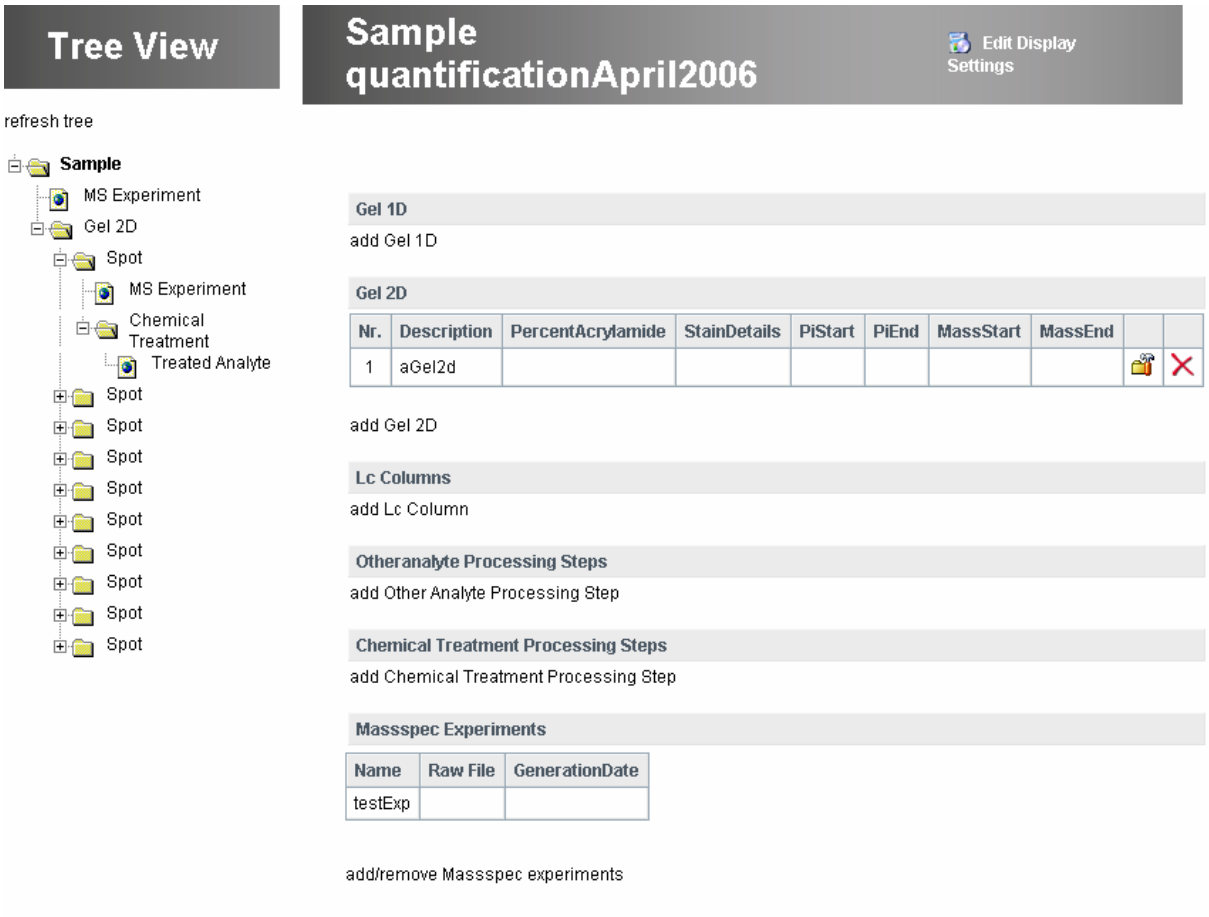
Here, information about the preparation steps of a sample can be entered.
First, you have to click on “Sample Generation->Sample->Find All Samples” and you get an overview of all your samples:



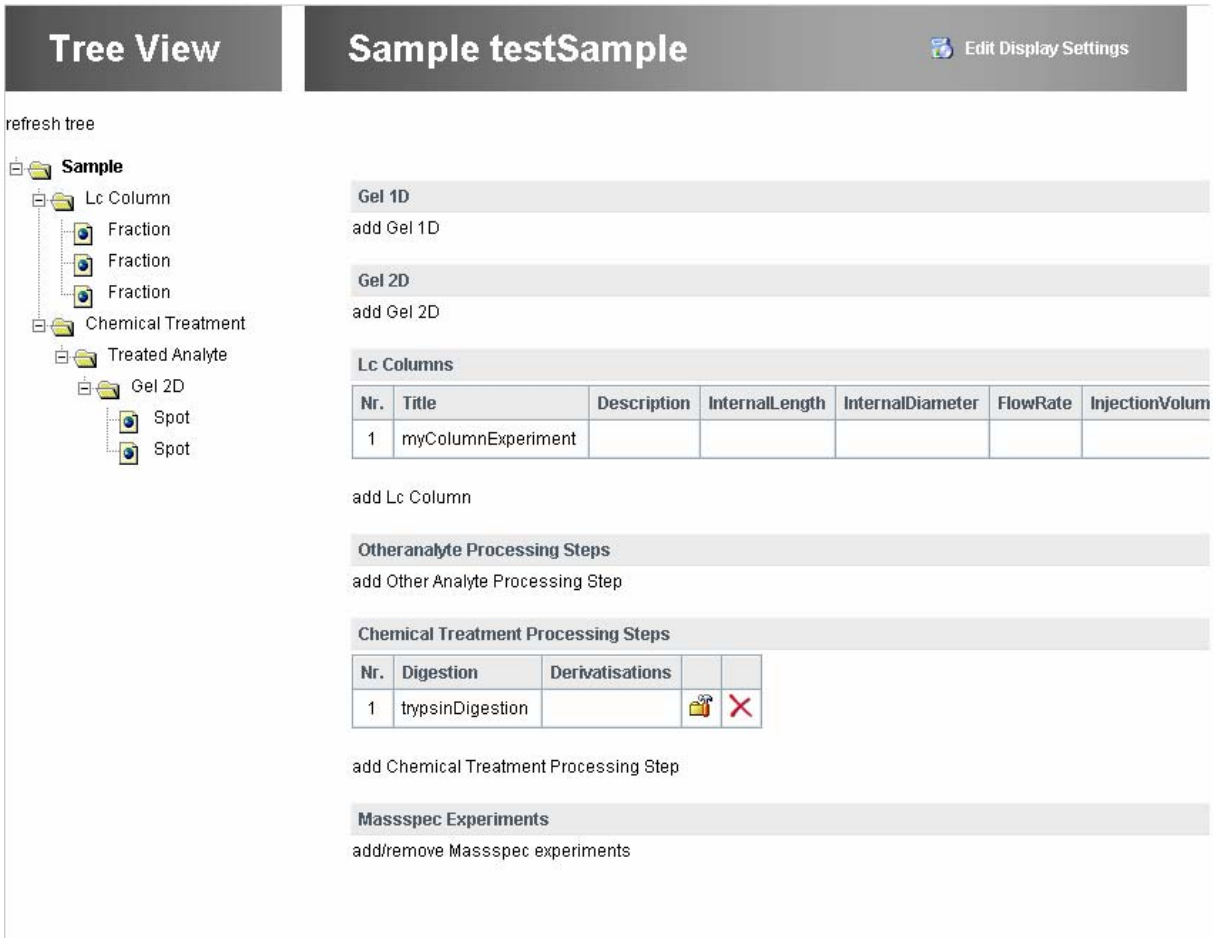
When you want to get more information on a sample, you click on the name for “sampleId” in the corresponding column to you reach the sample processing part. When you have a sample with no entries you will get the following page:



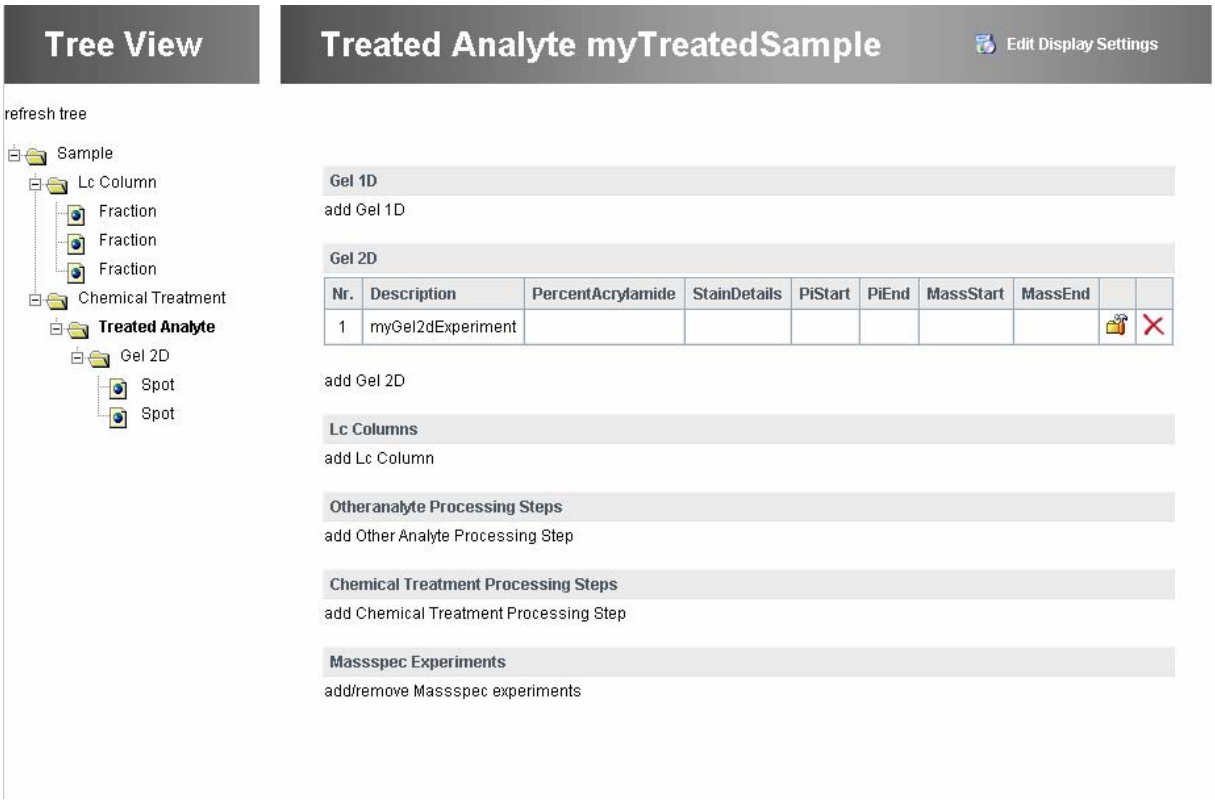
On the left side there should be a tree but now only the root element is there (the sample).
If you have entered values the page could look like the following:



The page splits into two parts, the tree view (see chapter 4.1 “Tree View”) and the information view where you can display and edit your data. You can arbitrarily manage your preparation steps here. E.g. you have a sample. With one half you ran it over an LC-Column, and got 3 Fractions which are interesting. The other half was first digested with trypsin and you got one treated analyte. With this one you made a 2D-Gel where you got a 2 interesting spots. Then the tree would look like the following:



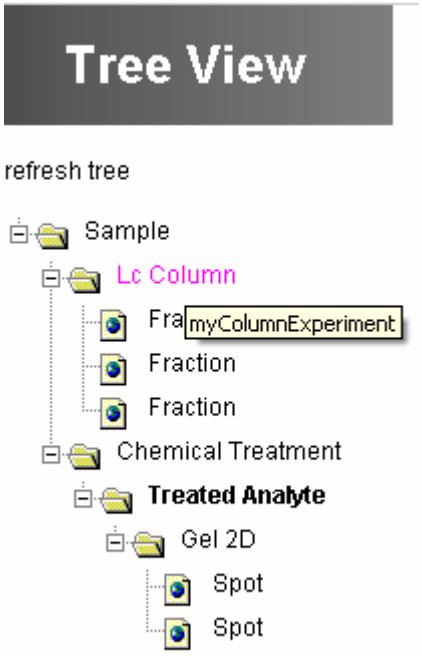
That means you can illustrate any splitting and any consecutive treatment. Regardless of the separation method you choose the organization is always the same. First you have a page where you can enter information about the separation method itself. After you have entered it once you can add with the edit option an arbitrary number of analytes. When you click on one of these analytes you will get again to a page where you can choose again between different analyte processing methods:



There are 5 different processing methods. A Gel1D leads to bands (for detailed information see chapter 4.2 Gel1D), a Gel2D leads to spots (for detailed information see chapter 4.3 Gel2D), a LC-Column leads to Fractions (for detailed information see chapter 4.4 LC-Column), a Chemical Treatment leads to Treated Analytes (for detailed information see chapter 4.5 Chemical Treatment), and Other Analyte Processing Steps (for detailed information see chapter 4.6 Other Analyte Processing Step) leads to Other Analytes. For all of the analytes Massspec experiments can be added (for detailed information how to add them see chapter 4.7 “Adding of Massspec experiments”). How you generate a Massspec Experiment see chapter 6.1 “Mass spectrometry experiment”.

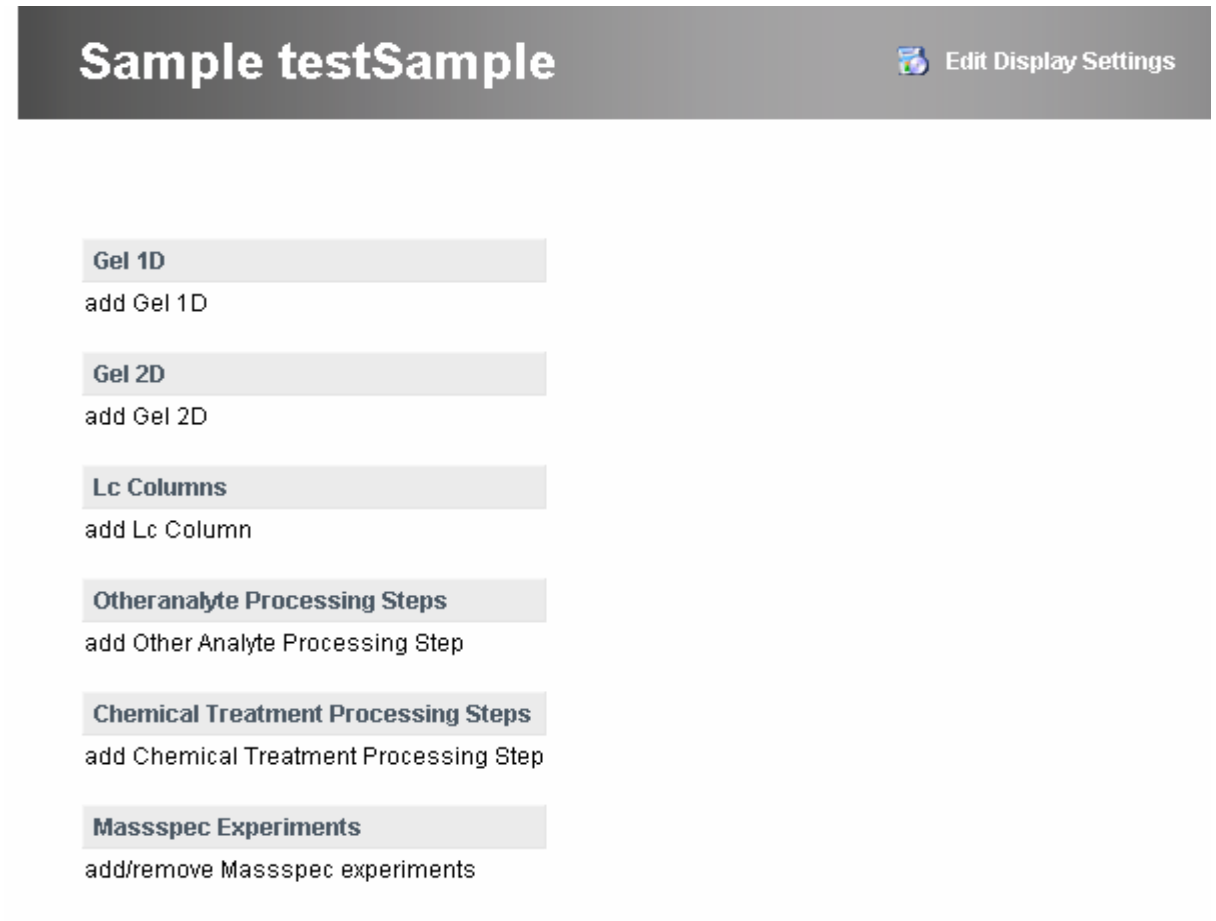
4.1 Tree view:

In the tree view the cross linking of the data is displayed graphically. In the tree the types of the analyte processing steps and the analytes are displayed. If you want to know the name of an element, you have to move your mouse over the element and a tool tip with the name will appear.

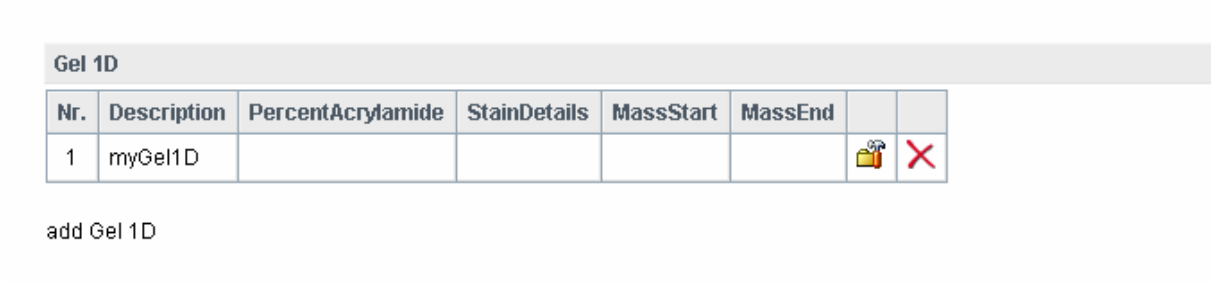


When you click on an element, information about this element will be displayed.
When you enter information on the right side the tree won't be updated automatically.
Press "refresh tree" to update it.

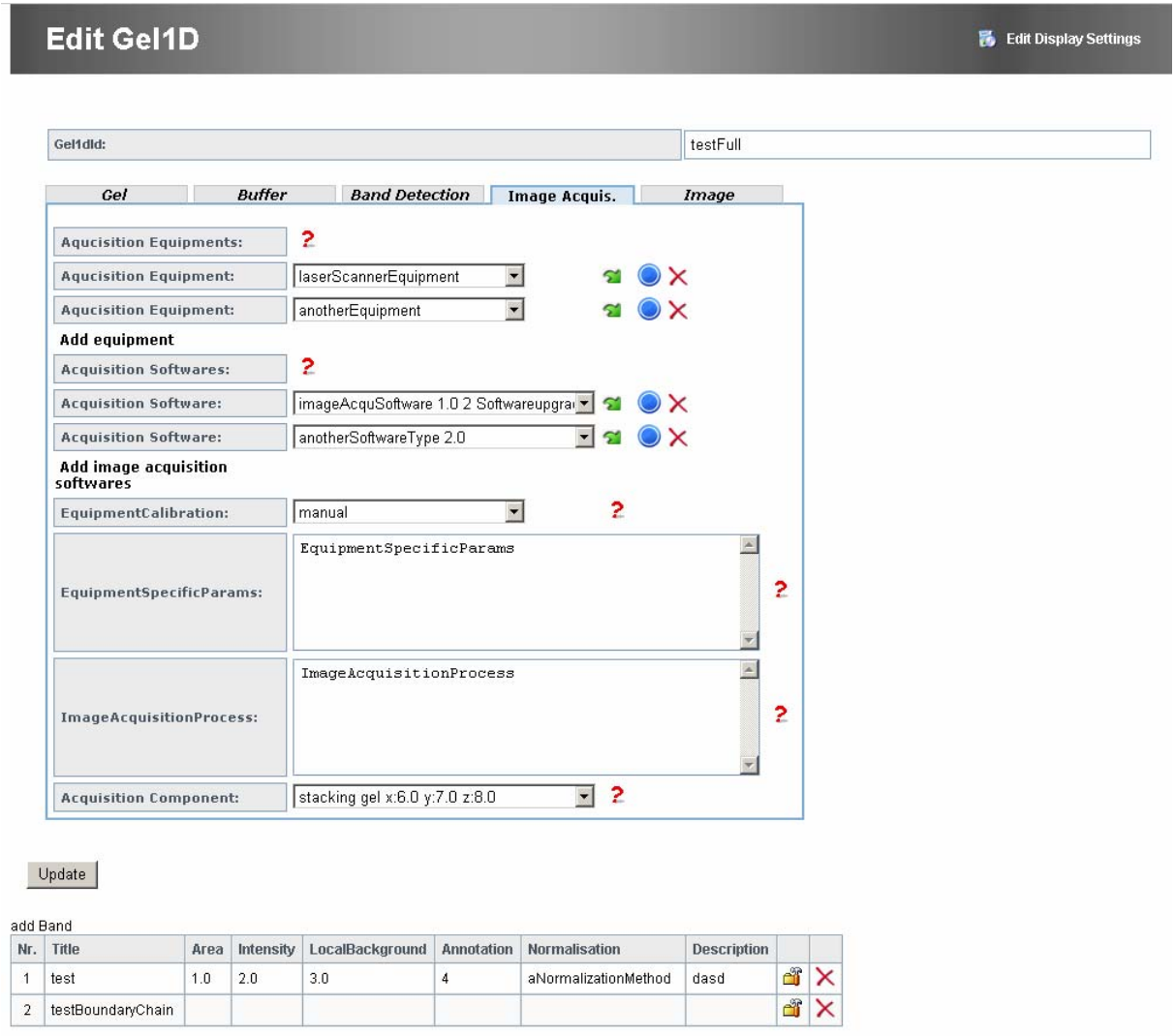
4.2 Gel1D:



When you are on the page of a sample or an analyte you can add a Gel1D with the link “add Gel 1D”. When you have added a Gel1D you will be redirected to the previous page displaying the added Gel1D.

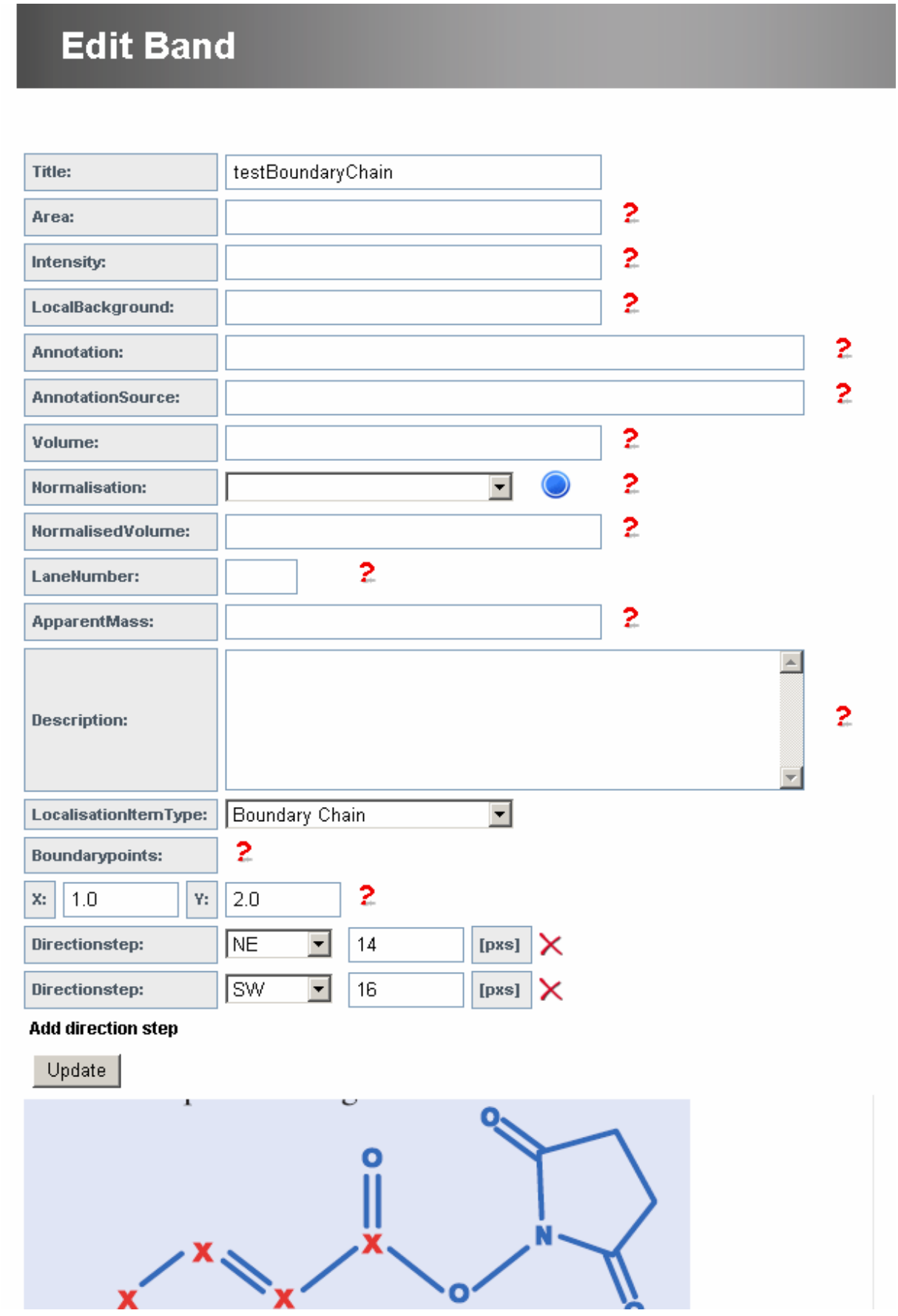


When you click on the description name or on the edit button you can edit it again.



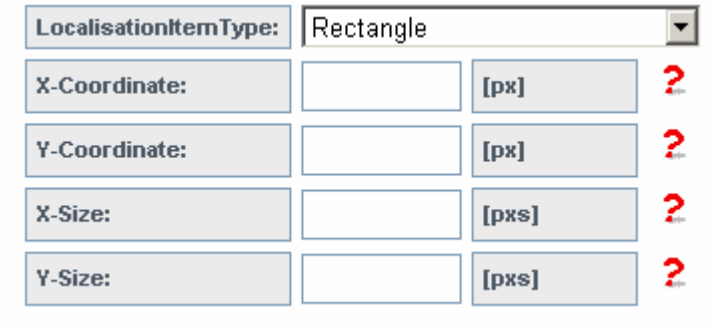
For the “Acquisition Component” you can select the whole selected “Gelmatrix” named with “Main” (you will find this select field, when you click on the “Gel” tab) or one of the components of the “Gelmatrix”. The references to the files (mostly images) which you can select in the “Image” tab, must be uploaded with the following upload types: Gel1D Raw Image for the Raw Image; Gel1D Warped Image for the Warped Image; Gel1D Warping Map for the Warping Map; Gel1D Annotated Image for the Annotated Image. All of the images can be displayed on this page as well.

Additionally to the create page link the “add Band” link for adding bands and a list with added bands will be displayed (here the edit page is shown).

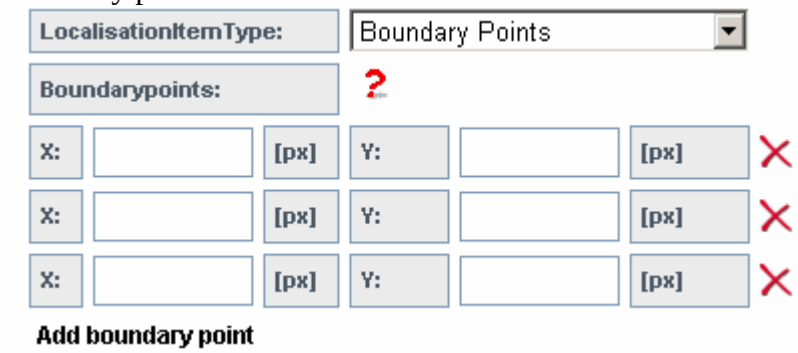


When you click on the edit or delete button of a band you reach this “create/edit” page again and you can make your changes, but by clicking on the title of the band (in this case “myBand”) you reach the page where you can add additional preparation steps or mass spectrometry experiments to the band.

At the bottom of the page the annotated image is shown (for demonstration purposes only an arbitrary image is shown). The localization of the band can be described in three different ways. The boundary chain is depicted in the image above.
Rectangle:

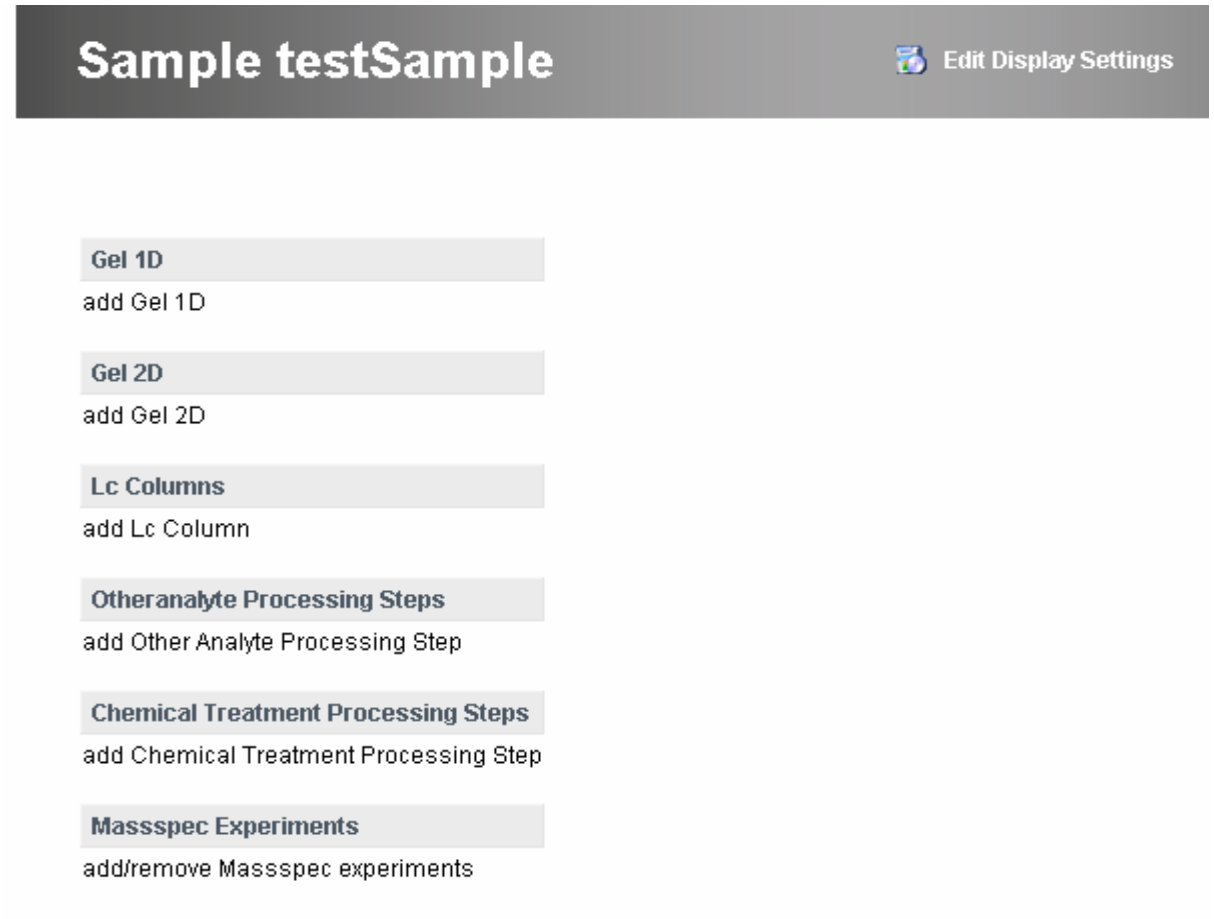


Boundary points:

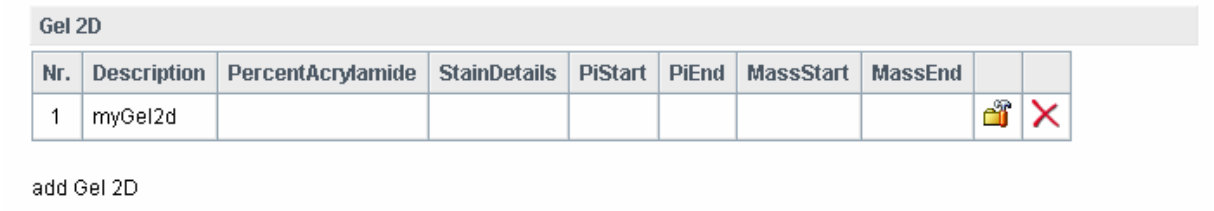


For the boundary chain and the boundary points the sequence of the entered values is important.

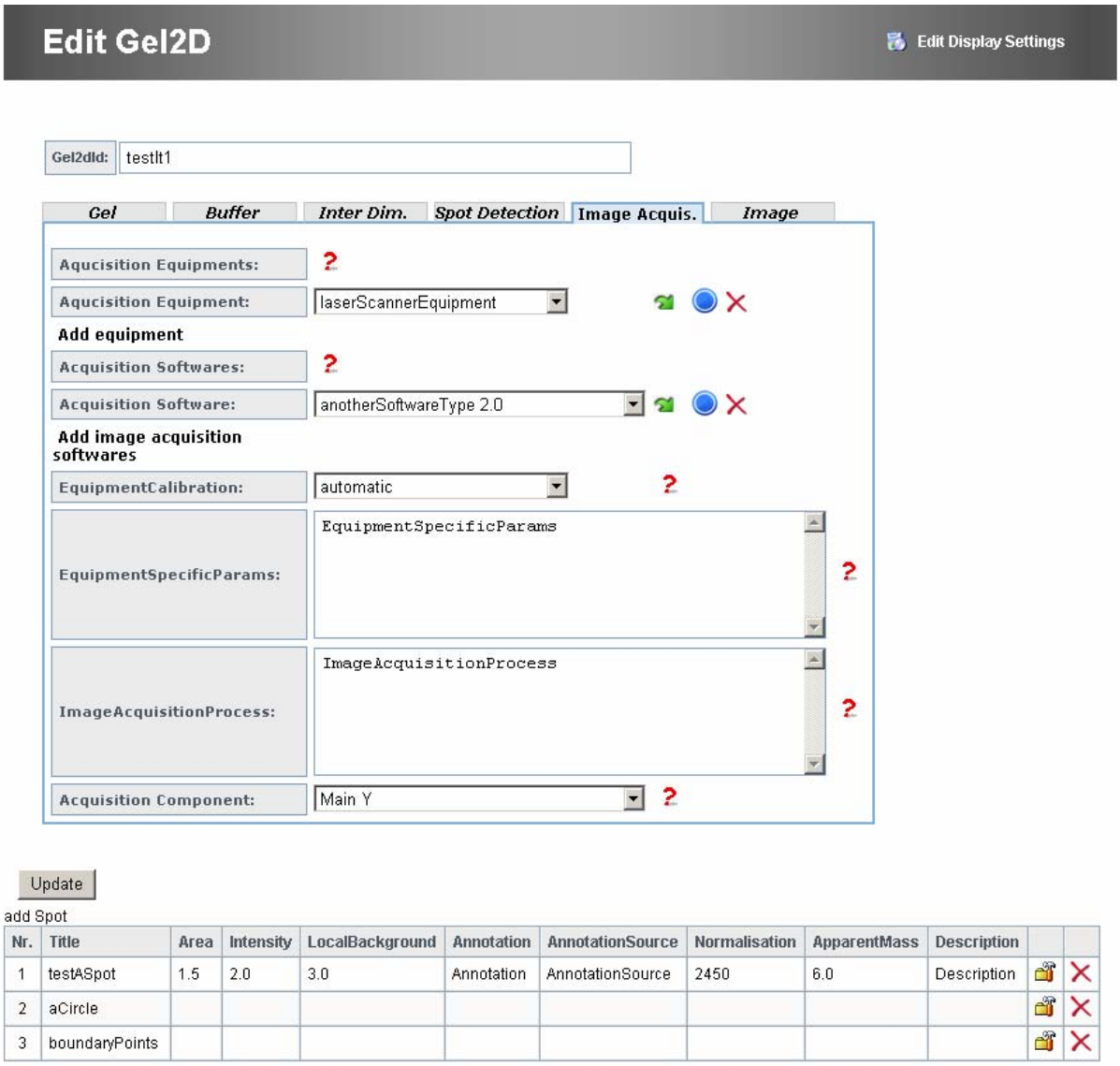
4.3 Gel2D:



When you are on the page of a sample or an analyte you can add a Gel2D with the link “add Gel 2D”. When you have added a Gel2D you will be redirected to the previous page containing the added Gel2D.

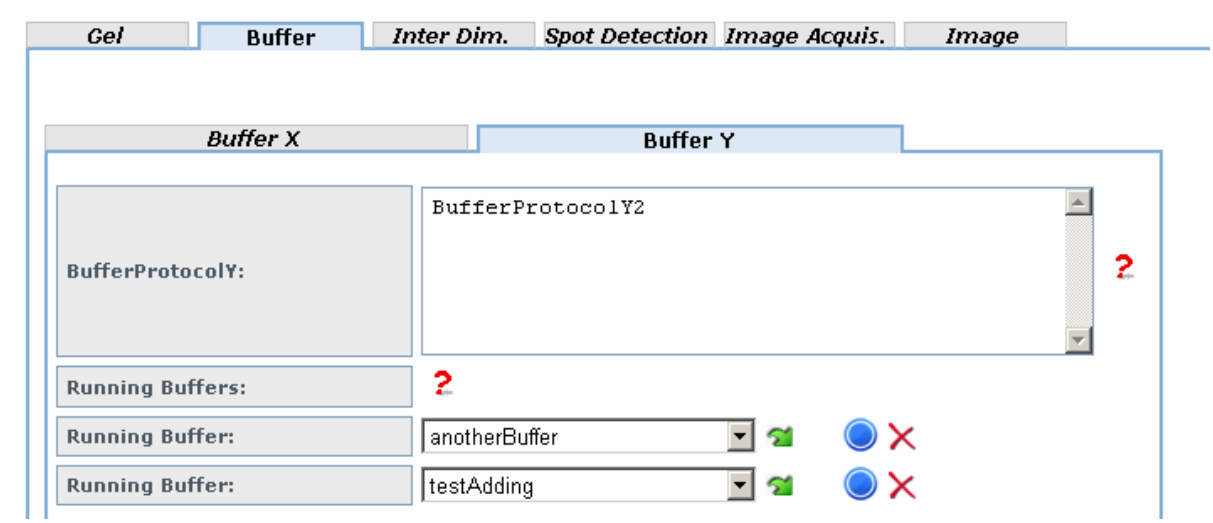


When you click on the description name or on the edit button you will be directed to the “create/edit” page again.

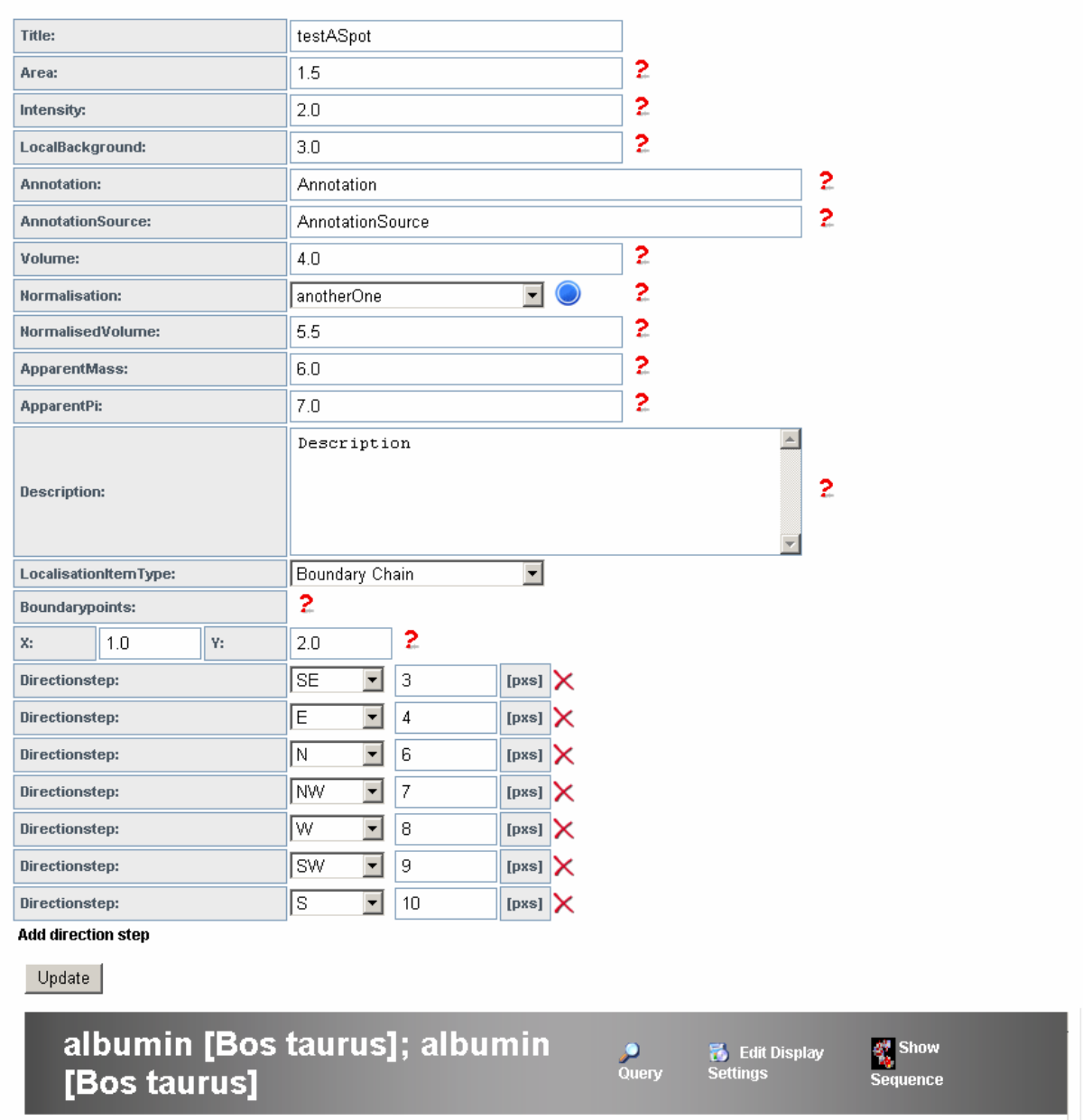


Nr.	Title	Area	Intensity	LocalBackground	Annotation	AnnotationSource	Normalisation	ApparentMass	Description		
1	testASpot	1.5	2.0	3.0	Annotation	AnnotationSource	2450	6.0	Description		
2	aCircle										
3	boundaryPoints										

For the “Acquisition Component” you can select the whole selected “Gelmatrix” for X and Y named with “Main X” and “Main Y” (you will find this select field, when you click on the “Gel” tab) or one of the components of the “Gelmatrix X” “Gelmatrix Y”. The references to the files (mostly images) which you can select in the “Image” tab, must be uploaded with the following upload types: Gel2D Raw Image for the Raw Image; Gel2D Warped Image for the Warped Image; Gel2D Warping Map for the Warping Map; Gel2D Annotated Image for the Annotated Image. All of the images can be displayed on this page as well. In contrast to the Gel1D the input mask is quite often divided by additional tabs in information concerning the X and concerning the Y section.



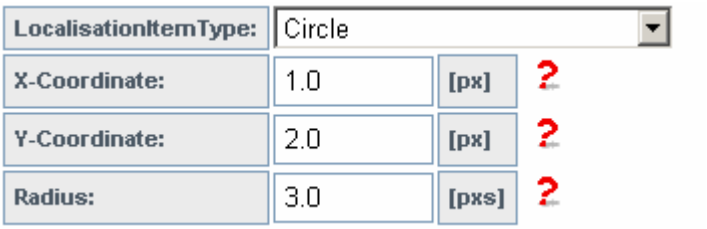
Additionally to the create page link the “add Spot” link for adding spots and a list with added spots will be displayed.



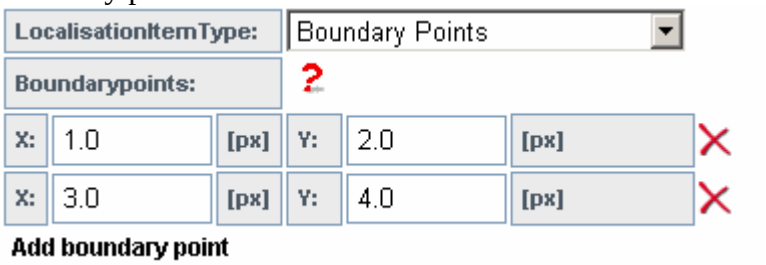
When you click on the edit or delete button of a spot you reach this “create/edit” page and you can make your changes, but by clicking on the title of the band (in this case “mySpot”) you reach the page where you can add additional preparation steps or mass spectrometry experiments to the spot.

At the bottom of the page the annotated image is shown (for demonstration purposes only an arbitrary image is shown). The localization of the spot can be described in three different ways. The boundary chain is depicted in the image above.

Circle:

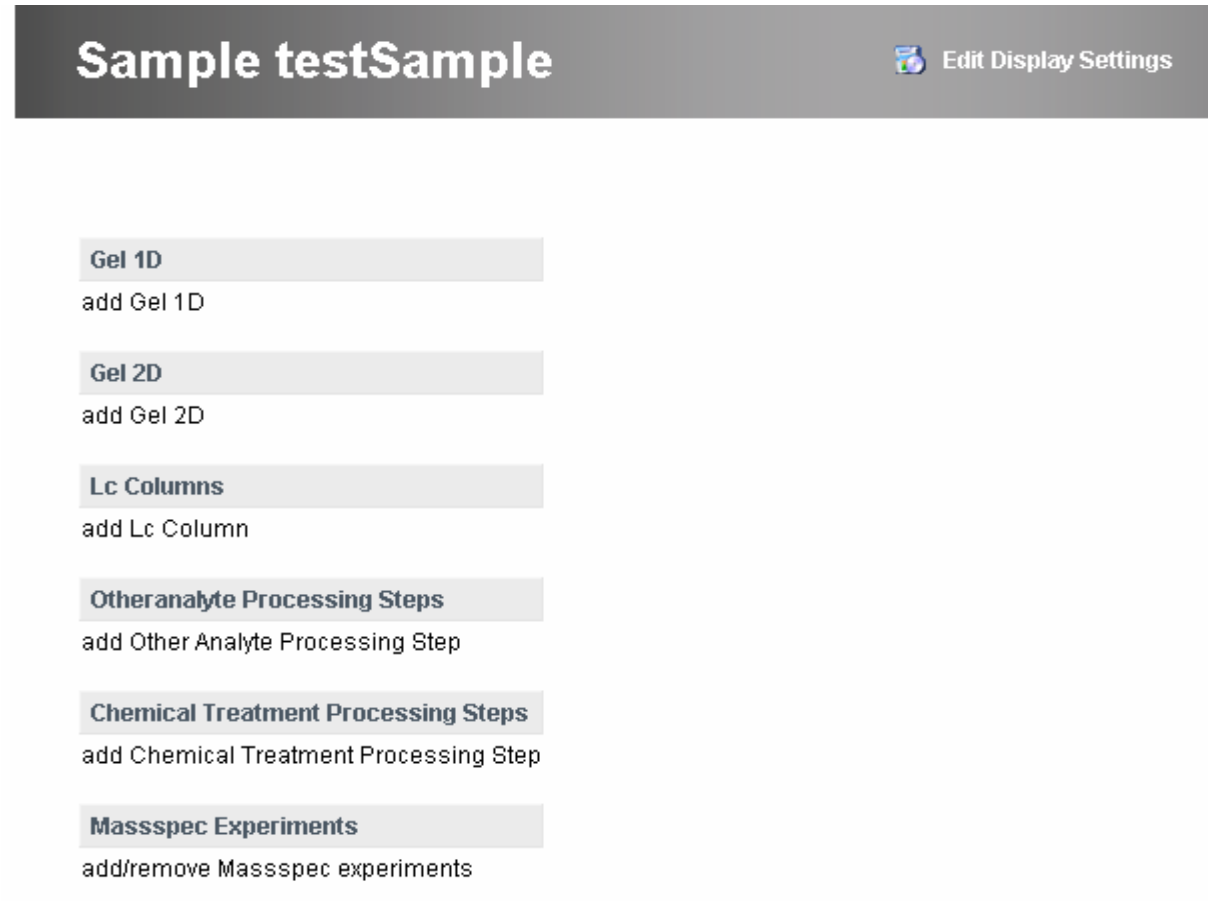


Boundary points:

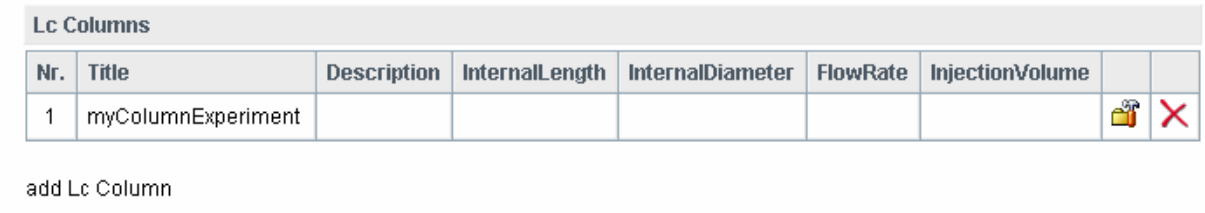


For the boundary chain and the boundary points the sequence of the entered values is important.

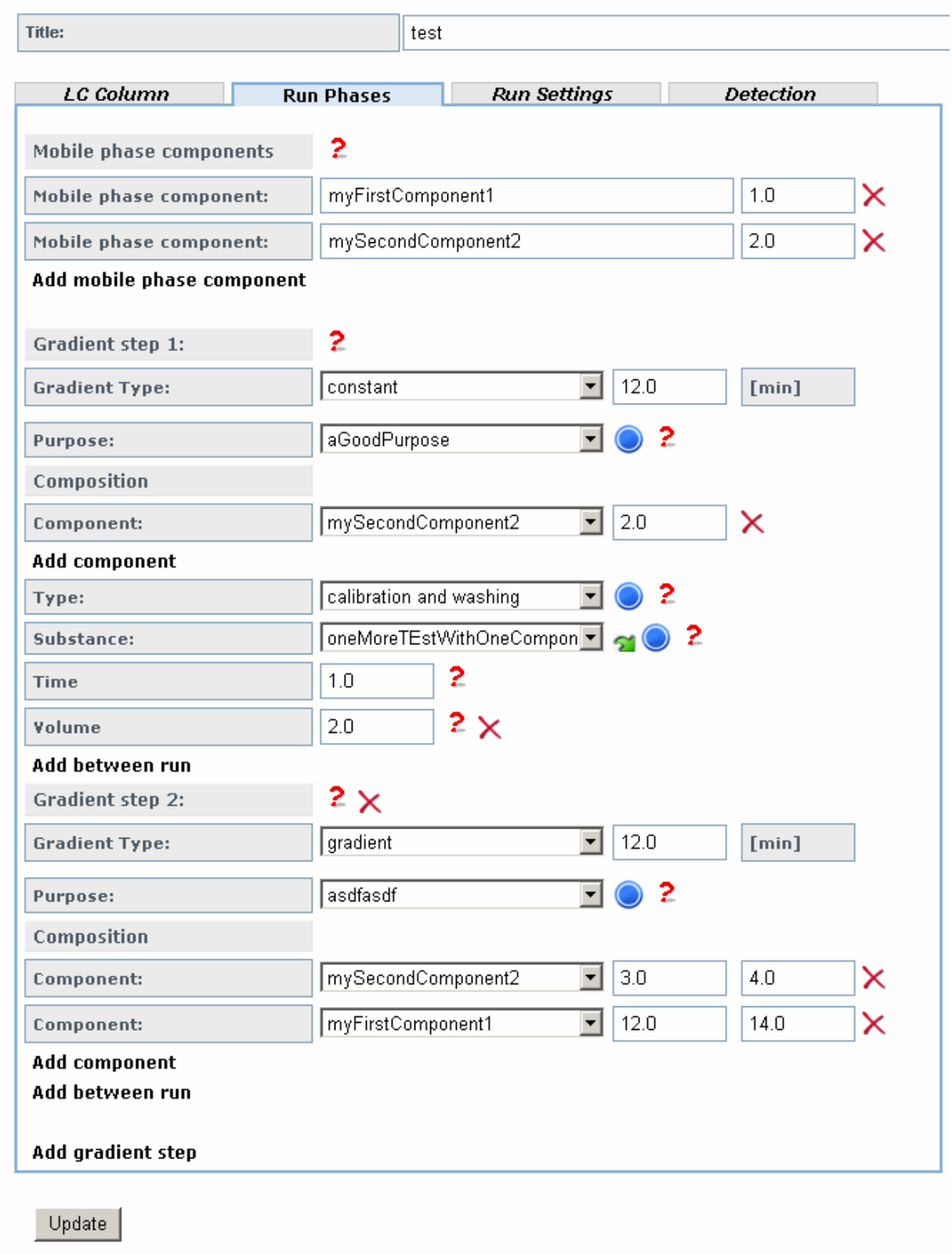
4.4 LC-Column:



When you are on the page of a sample or an analyte you can add a LC-Column with the link “add Lc Column“. When you have added an LC-Column you will be redirected to the previous page containing the added LC-Column.

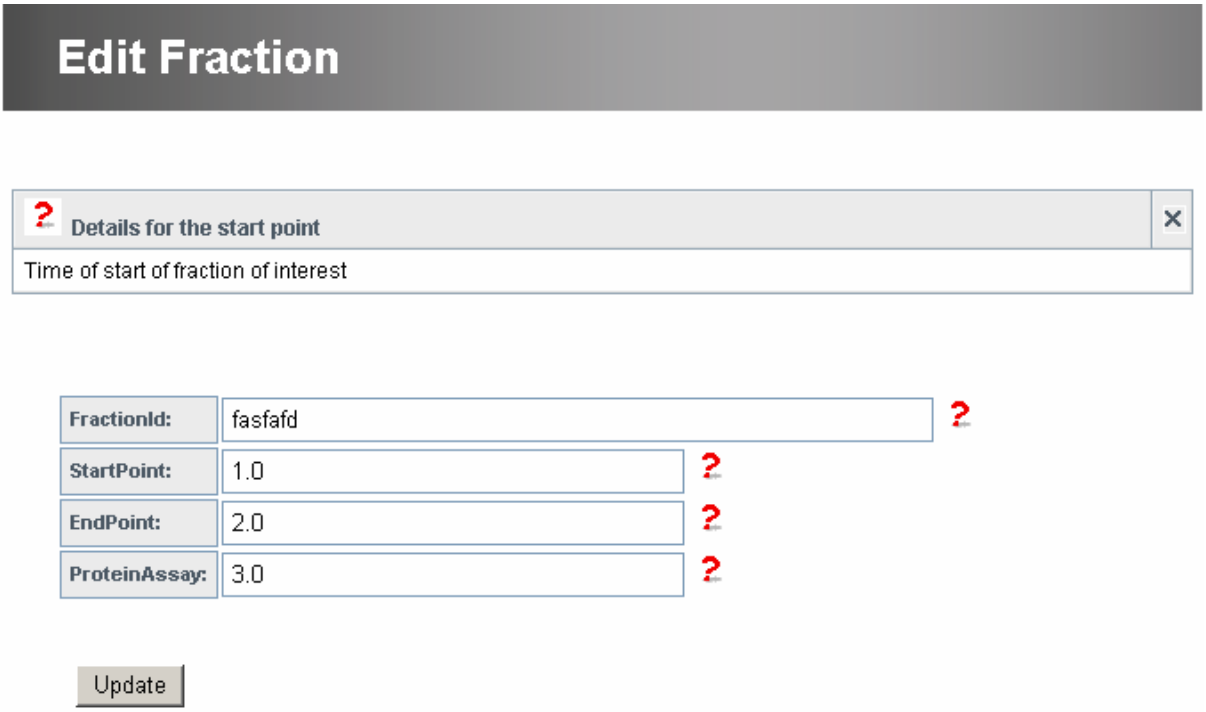


When you click on the title name or on the edit button you will be directed to “create/edit” page again.



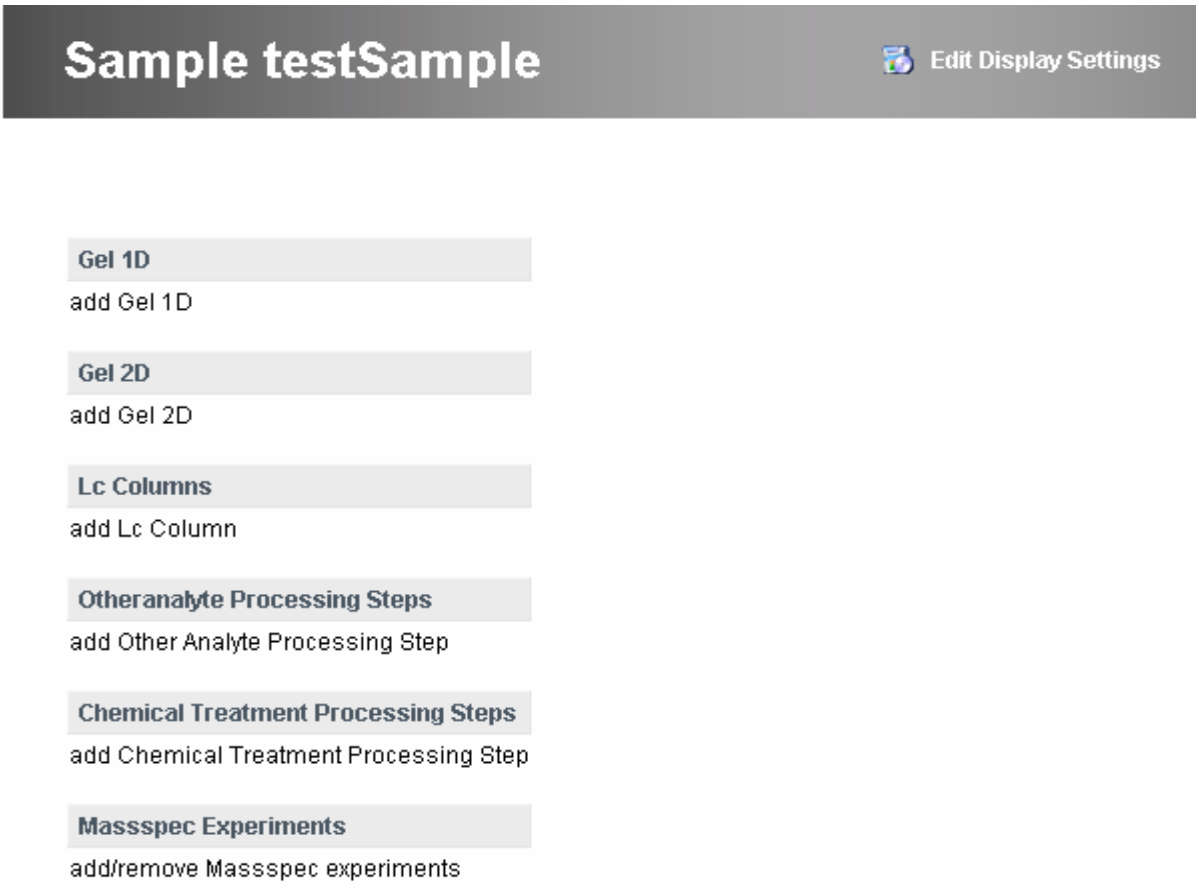
In this page you can enter different mobile phase components, which you can select (after entering) in the component select field.

Additionally to the create page link the “add Fraction” link for adding fractions and a list with added fractions will be displayed.



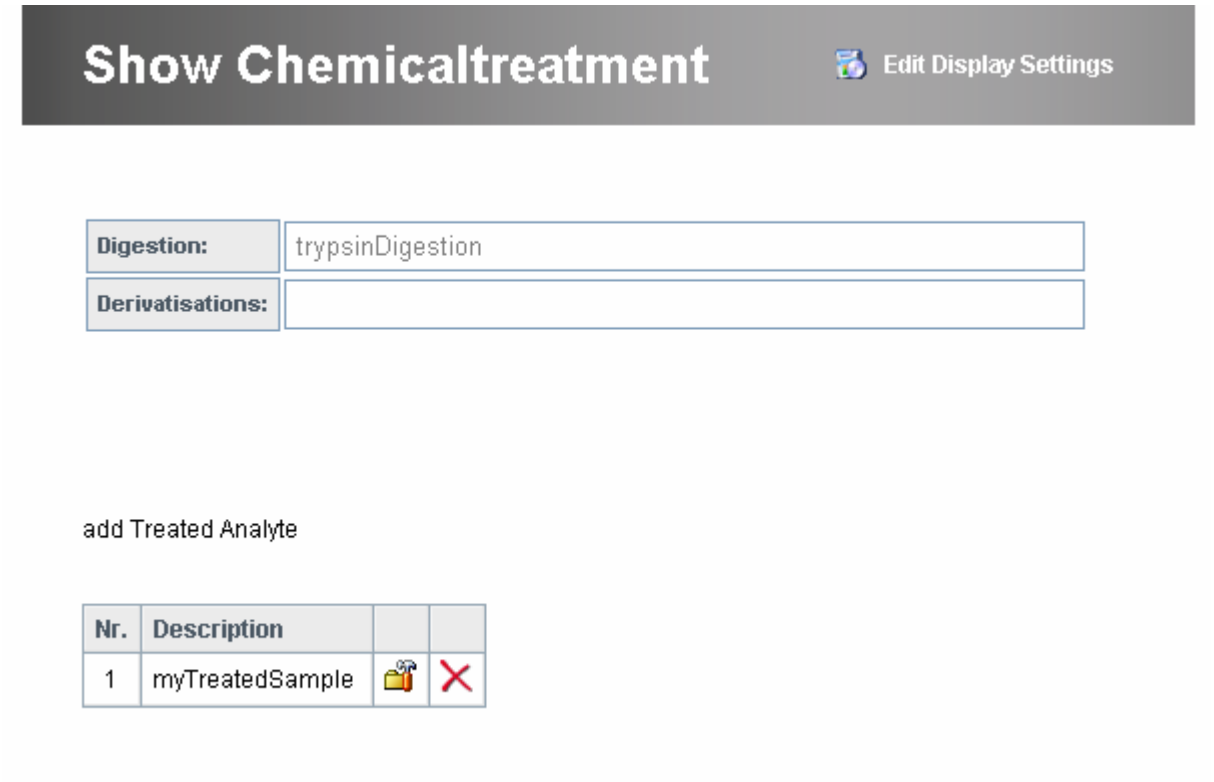
When you click on the edit or delete button of a Fraction you reach this “create/edit” page and you can make your changes, but by clicking on the title of the fractionId (in this case “firstFraction”) you reach the page where you can add additional preparation steps or mass spectrometry experiments to the fraction.

4.5 Chemical Treatment:

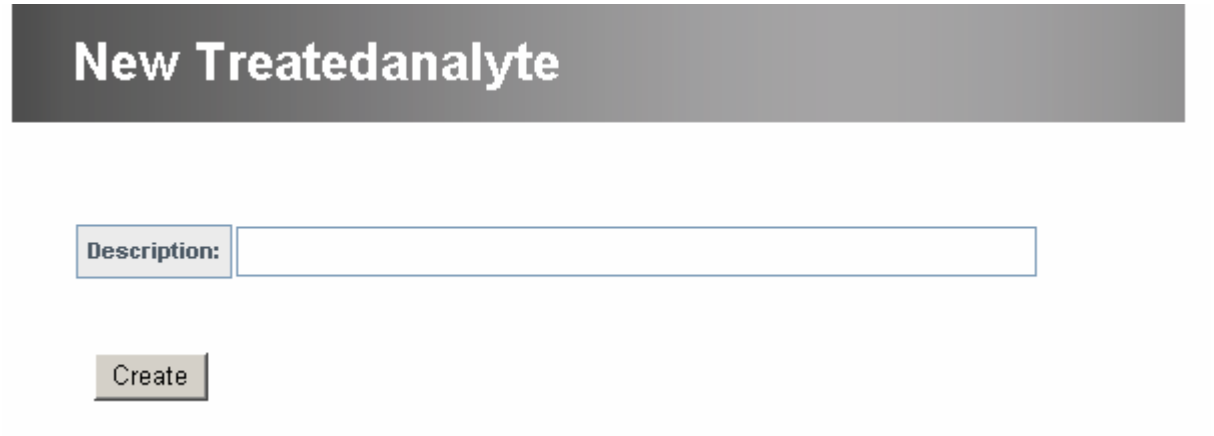


When you are on the page of a sample or an analyte you can add chemical treatments with the "add Chemical Treatment Processing Step"link. When you have added a chemical treatment you will be redirected to the previous page containing the added chemical treatment.

When you click on the digestion name or on the edit button you will be directed to the same "create/edit" page again.

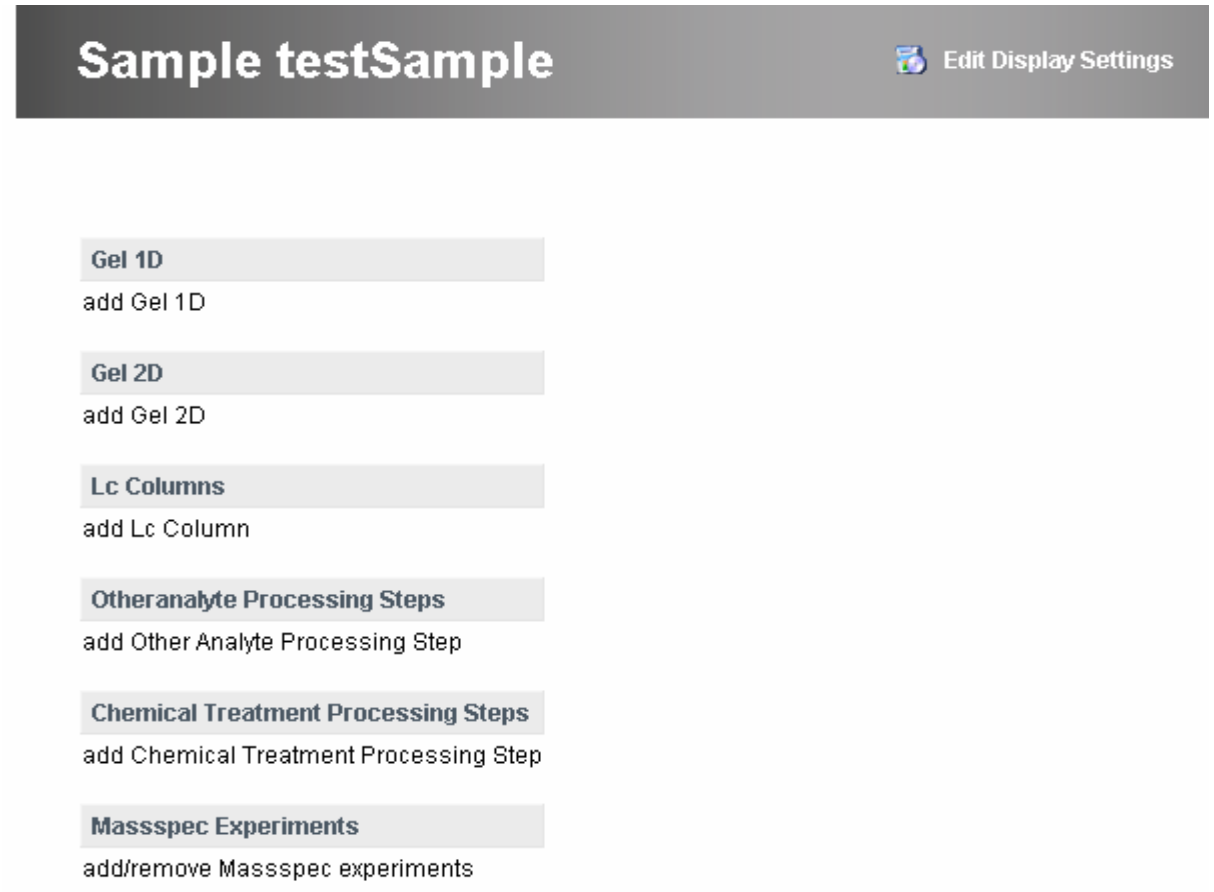


Additionally to the create page link the “add Treated Analyte” link for adding treated analytes and a list with added treated analytes will be displayed.

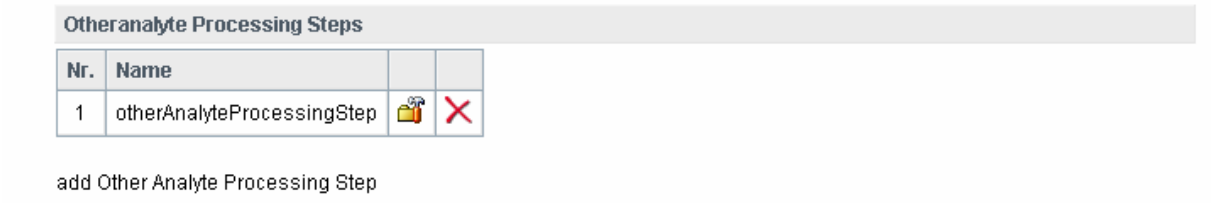


When you click on the edit or delete button of an treated analyte you reach this “create/edit” page again and you can make your changes, but by clicking on the name of the description (in this case “myTreatedSample”) you reach the page where you can add additional preparation steps or mass spectrometry experiments to the treated analyte.

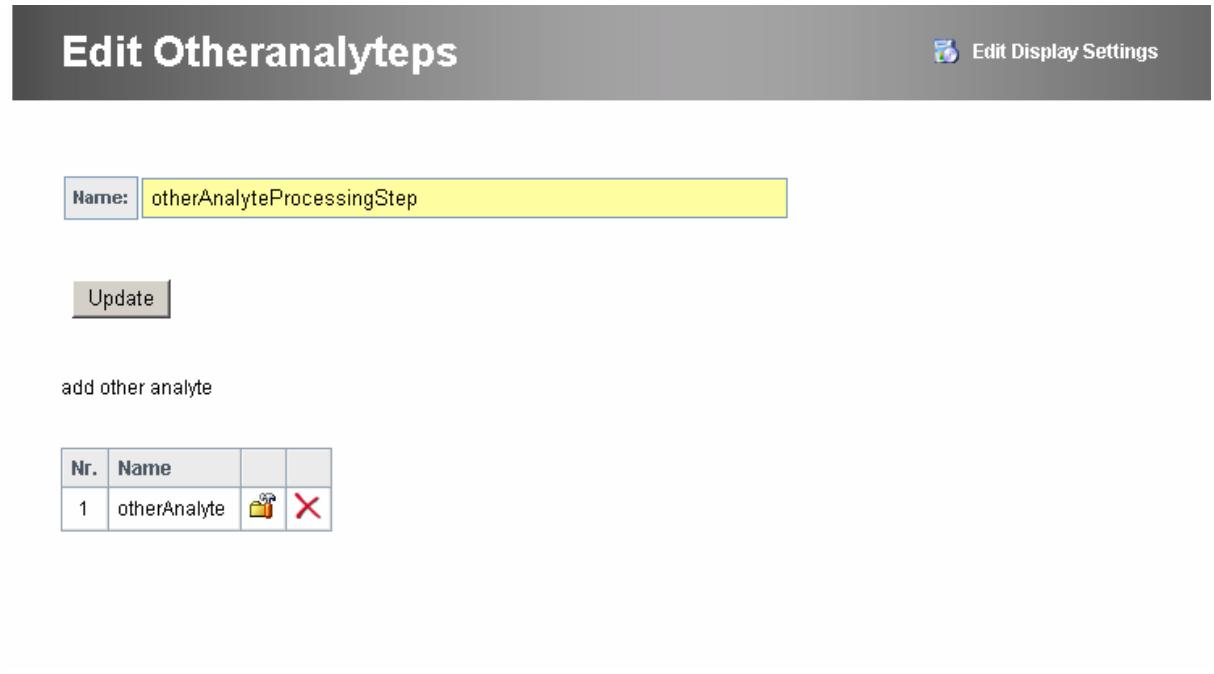
4.6 Other Analyte Processing Step:



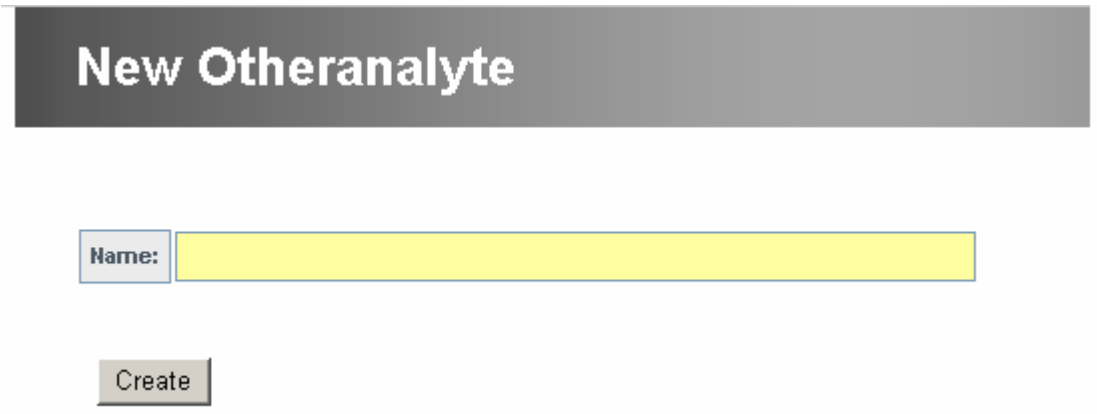
When you are on the page of a sample or an analyte you can add other analyte processing steps with the link “add Other Analyte Processing Step“. When you have added an other analyte processing step you will be redirected to the previous page containing the added other analyte processing step.



When you click on the name or on the edit button you will be directed to the same “create/edit” page again.

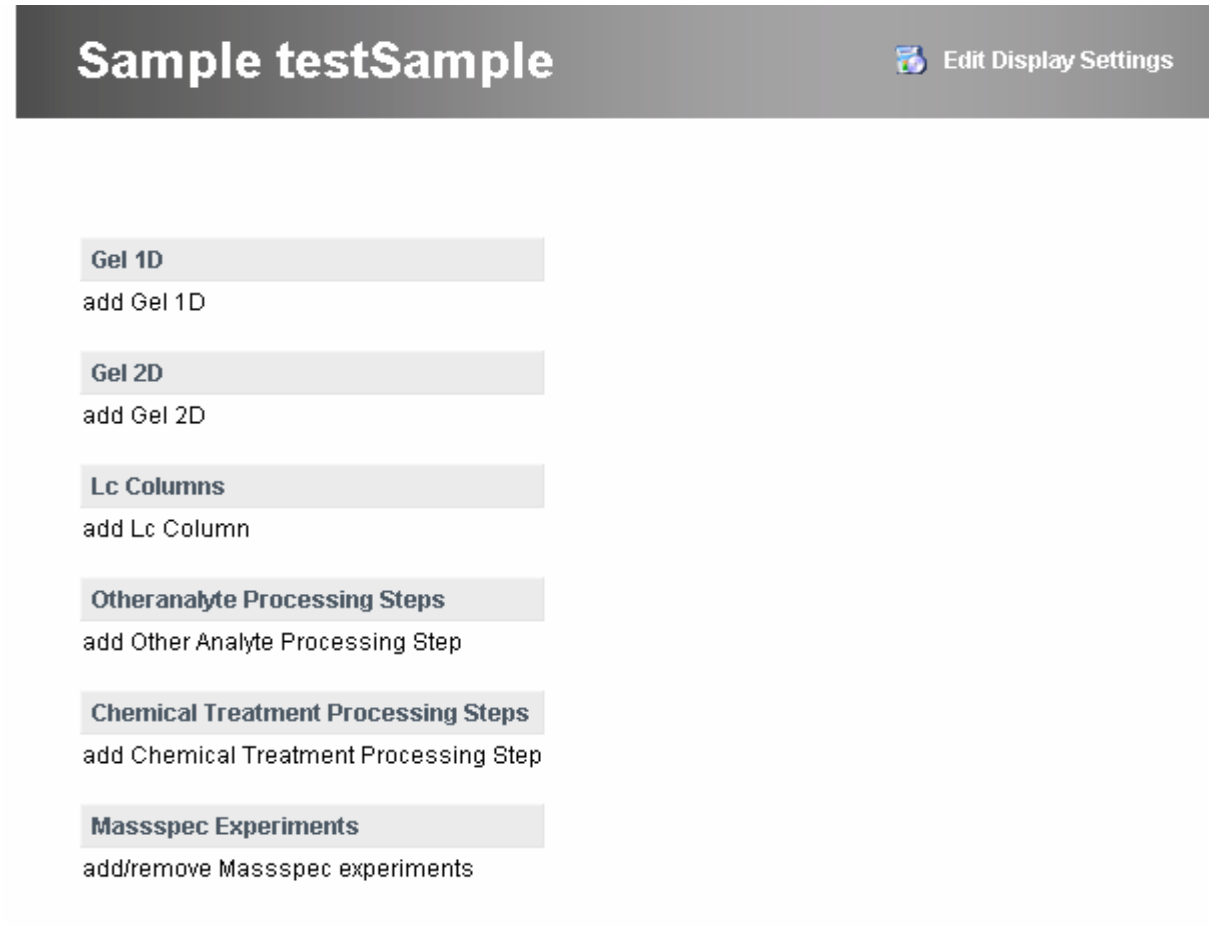


Additionally to the create page link the “add other analyte” link for adding other analytes and a list with added other analytes will be displayed.

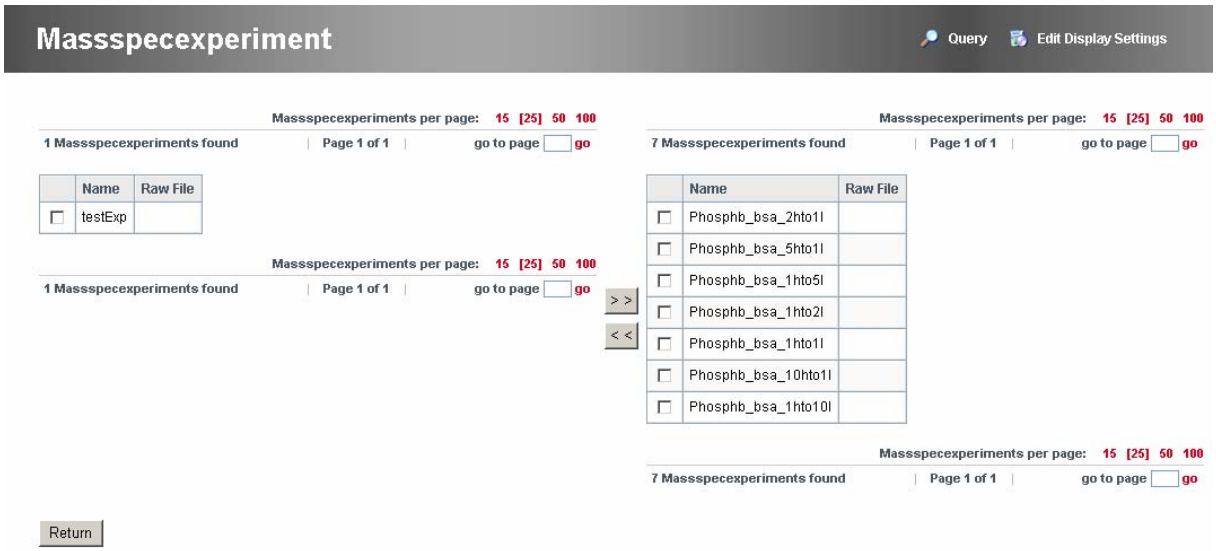


When you click on the edit or delete button of an analyte you reach this “create” page and you can make your changes, but by clicking on the name (in this case “otherAnalyte”) you reach the page where you can add additional preparation steps or mass spectrometry experiments to the otherAnalyte.

4.7 Adding of Massspec experiments



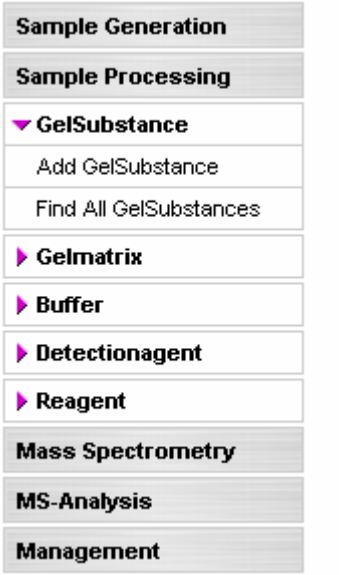
When you have added some mass spectrometry experiments, there is a direct link on the title of the mass spectrometry experiment to the mass spectrometry experiment.
When you are on the page of a sample or an analyte you can add other mass spectrometry experiments using the “add/remove Massspec experiments“link.



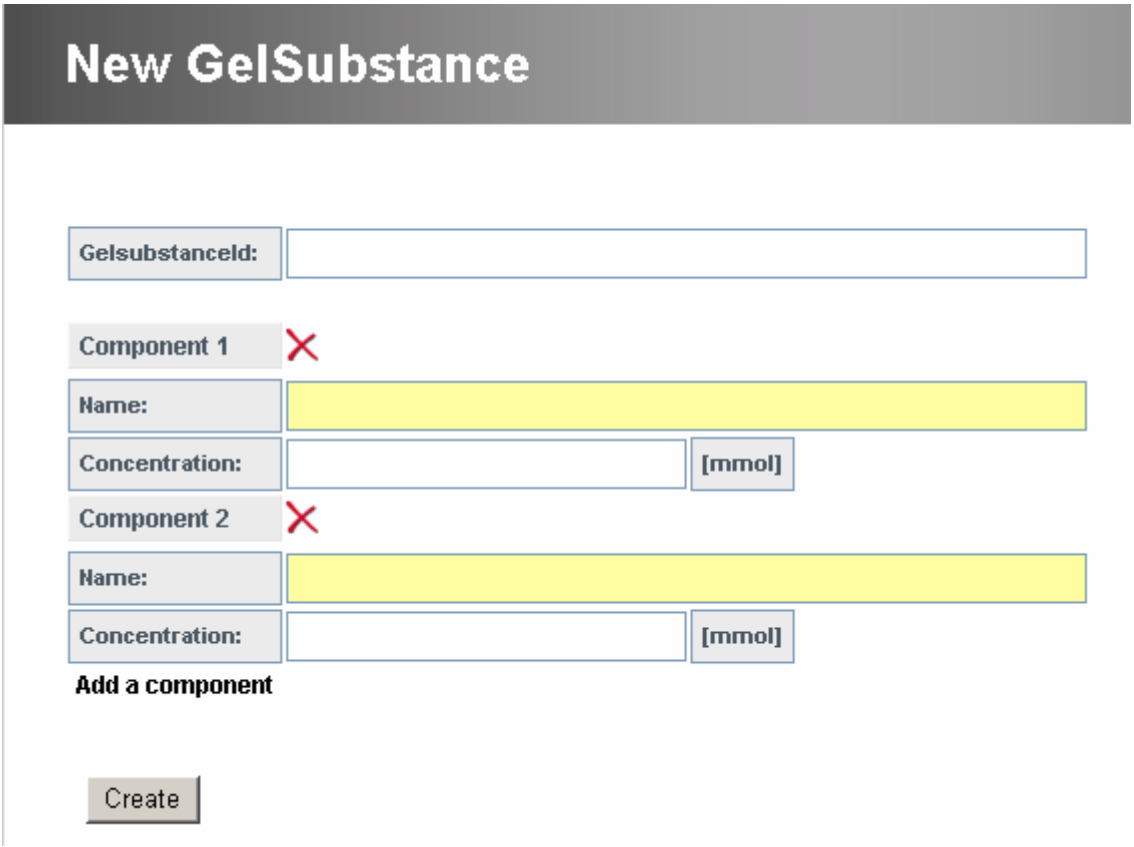
Adding massspec experiments to an analyte works the same way as adding samples to experiments (see chapter 3.2.2). The only difference is that only those mass spectrometry experiments are displayed on the left side, which are not already added to an analyte, while the sample can be added to several experiments. For detailed information how to create mass spectrometry experiments see 6.1 “Mass spectrometry experiment”.

4.8 Gel Substance

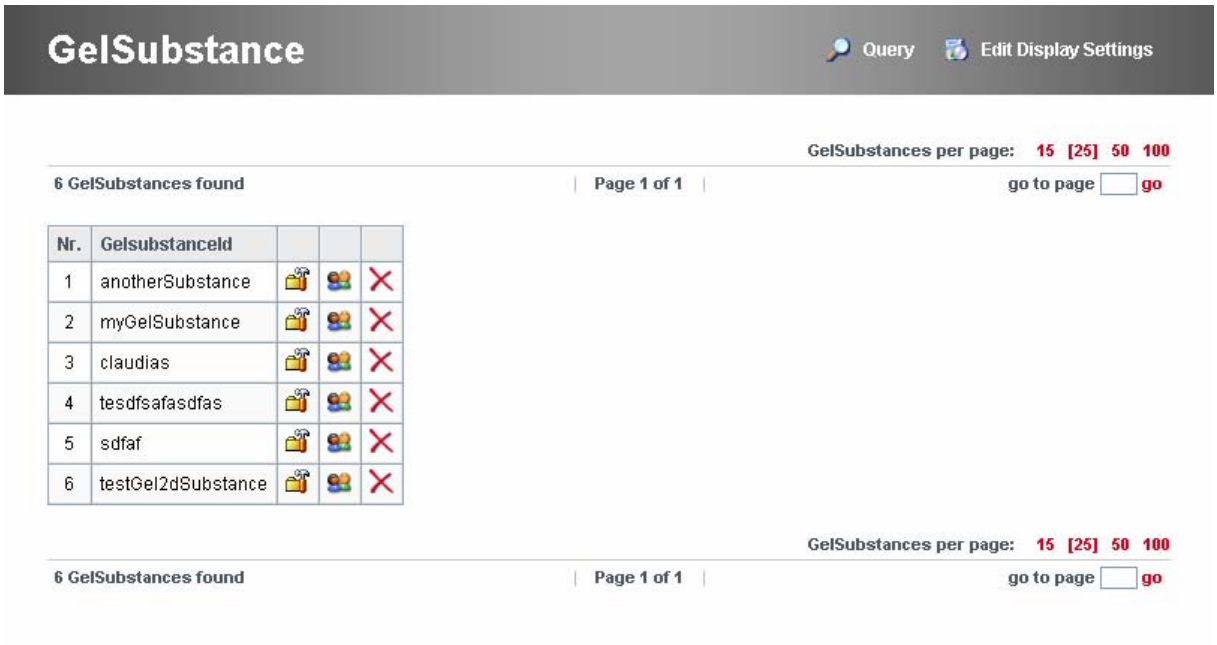
By clicking Sample Processing->GelSubstance you reach gel substance section.



With the “Add GelSubstance” you can add gel substances.



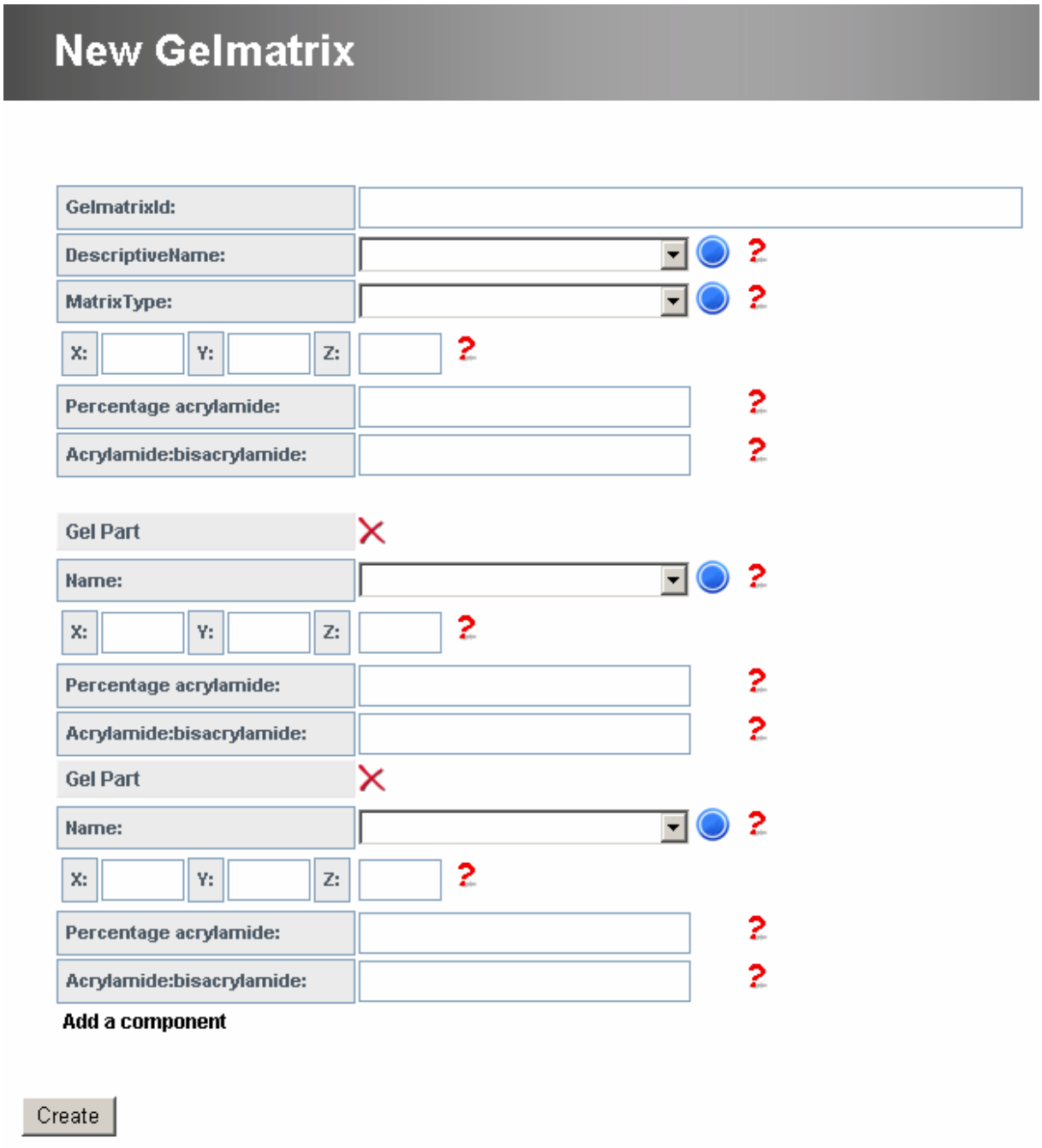
With a click on the button “Find All GelSubstances” you get an overview of all your gel substances:



4.9 Gel Matrix

By clicking Sample Processing->Gelmatrix you reach gel matrix section.

With the “Add Gelmatrix” you can add gel matrices.

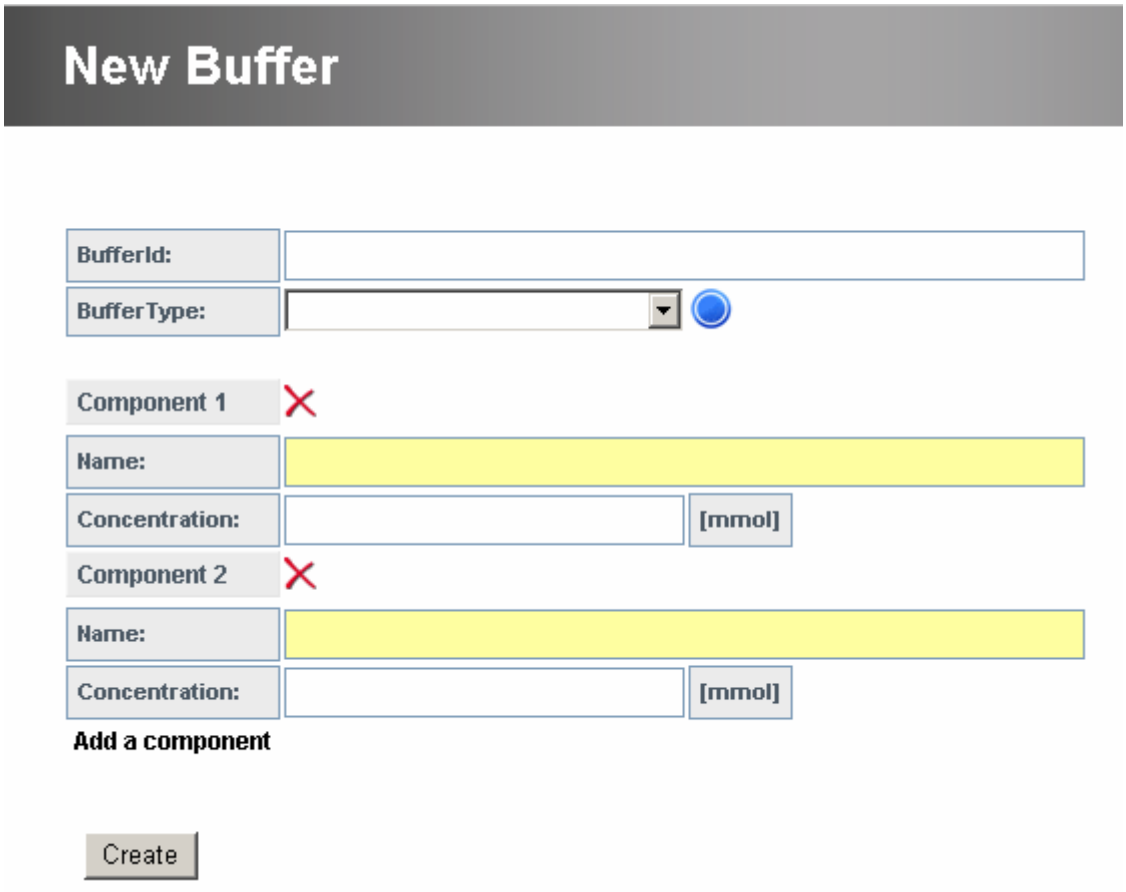


With a click on the button “Find All Gelmatrices” you get an overview of all your gel matrices:

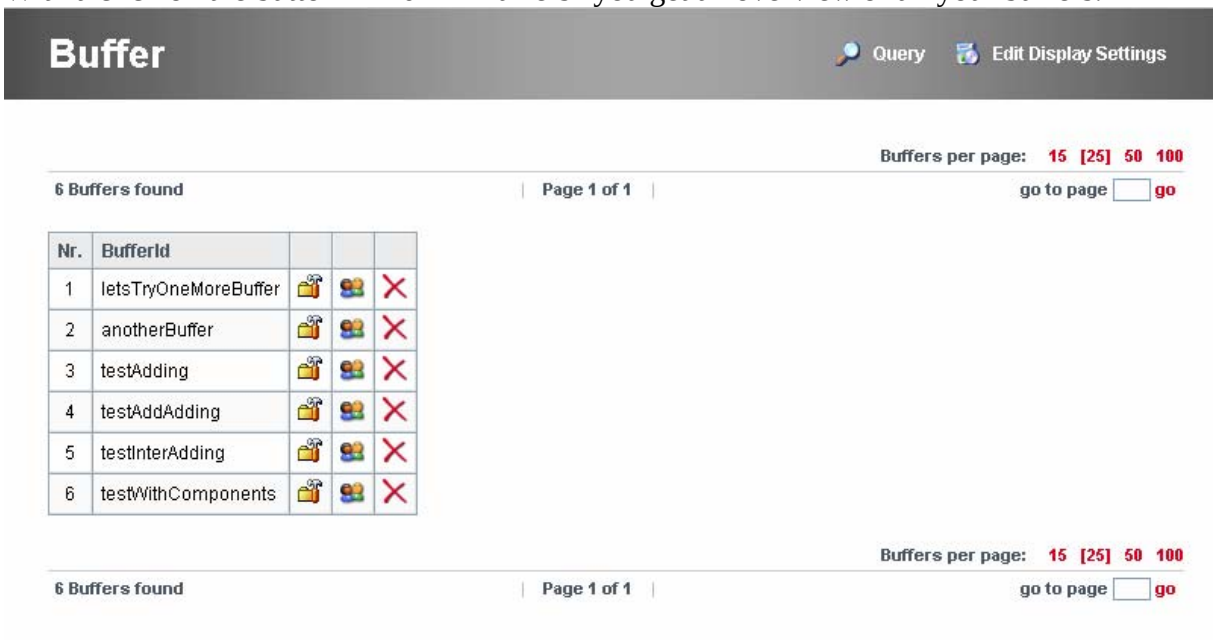
4.10 Buffer

By clicking Sample Processing->Buffer you reach buffer section.

With the “Add Buffer” you can add buffers.

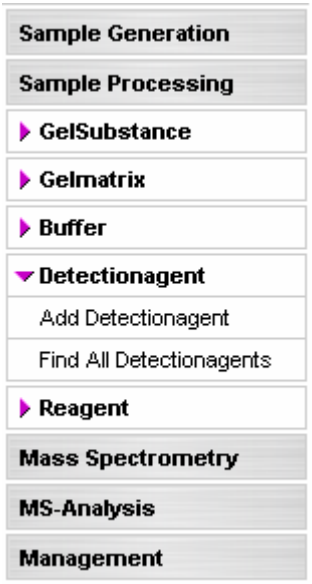


With a click on the button “Find All Buffers” you get an overview of all your buffers:

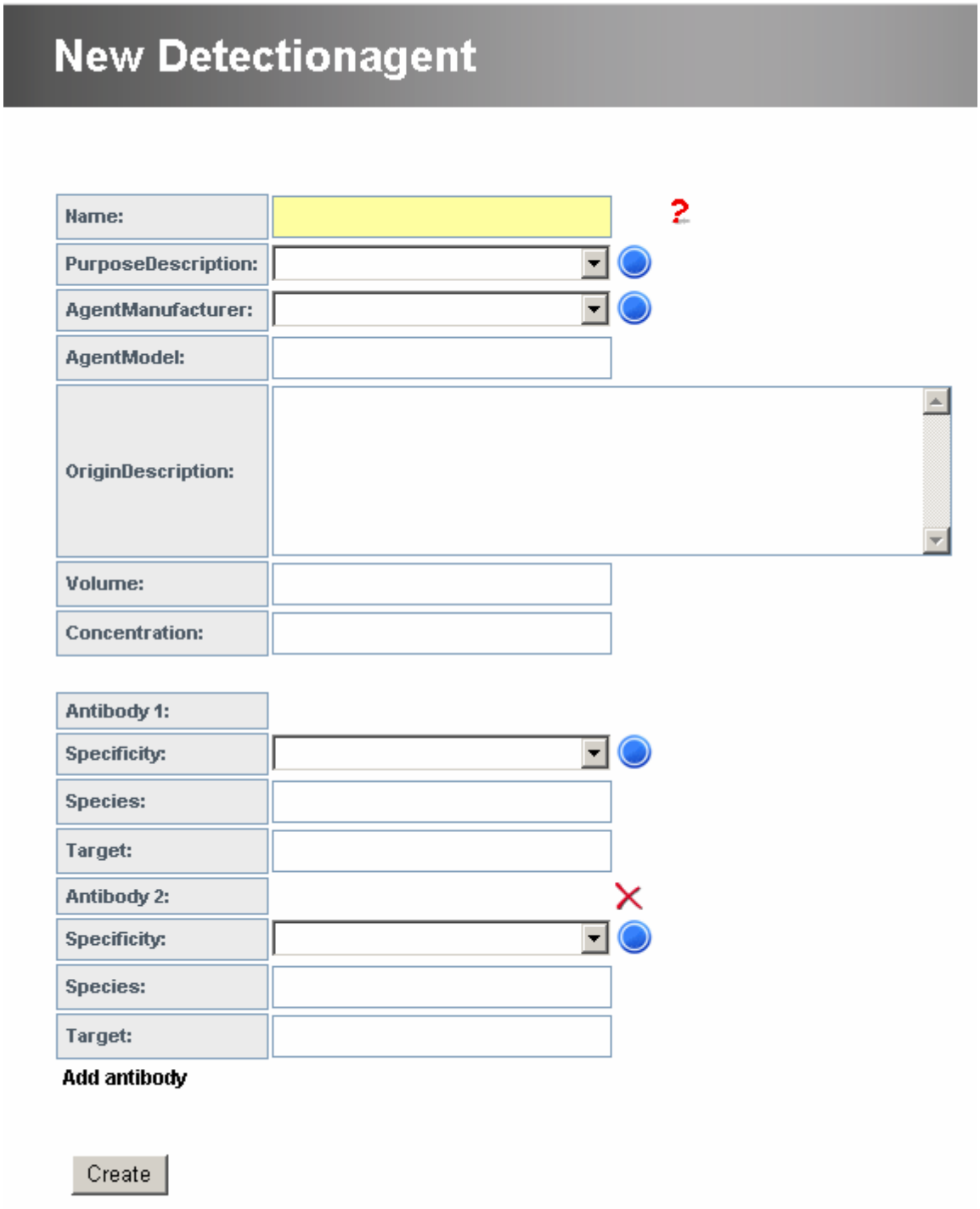


4.11 Detection agent

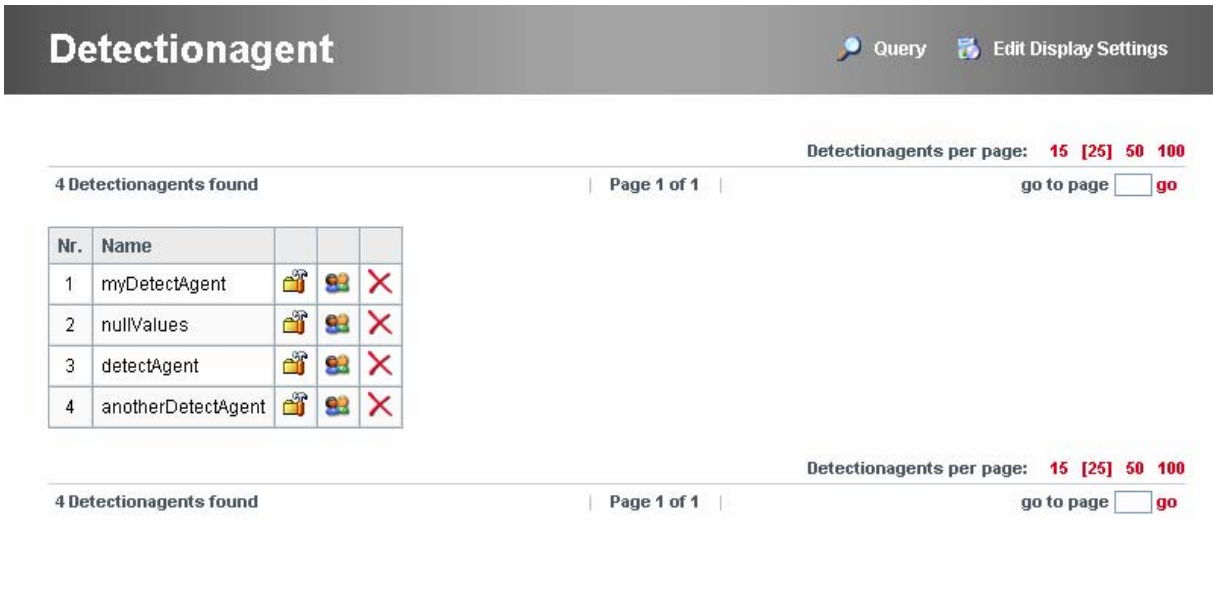
By clicking Sample Processing->Detectionagent you reach detection agent section.



With the “Add Detectionagent” you can add detection agents.



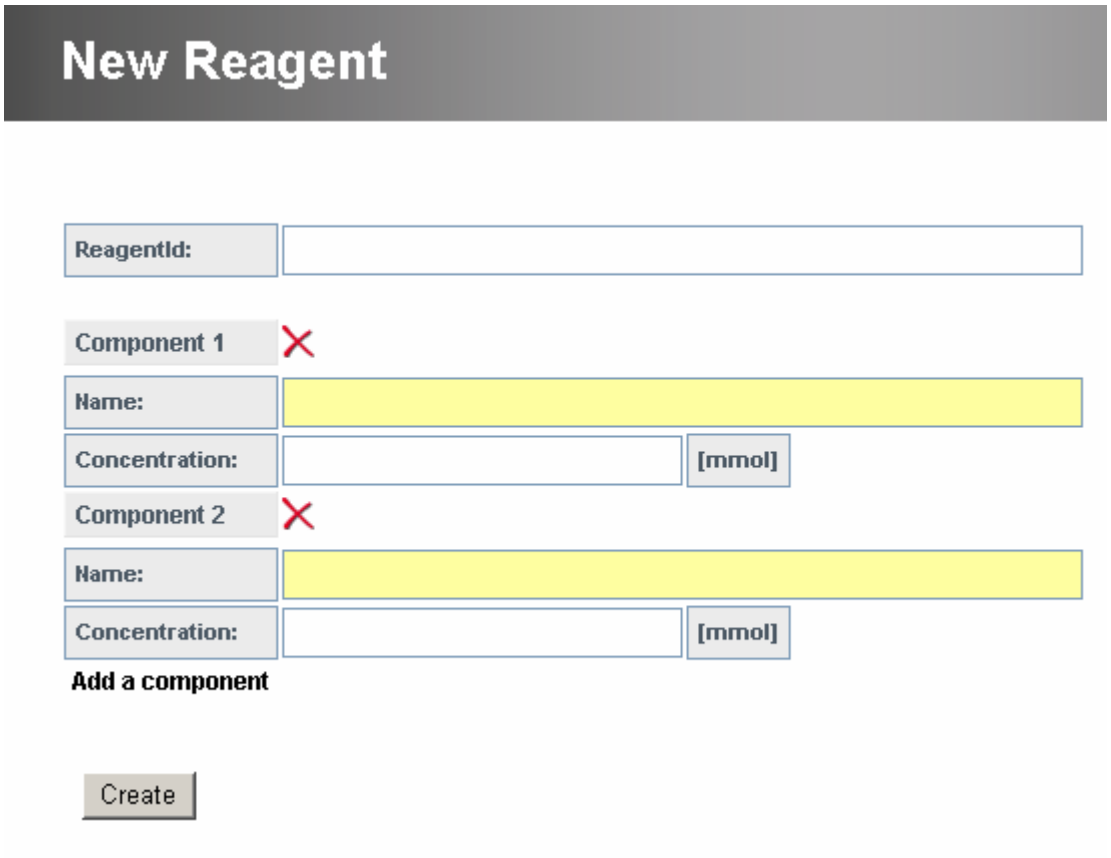
With a click on the button “Find All Detectionagents” you get an overview of all your detection agents:



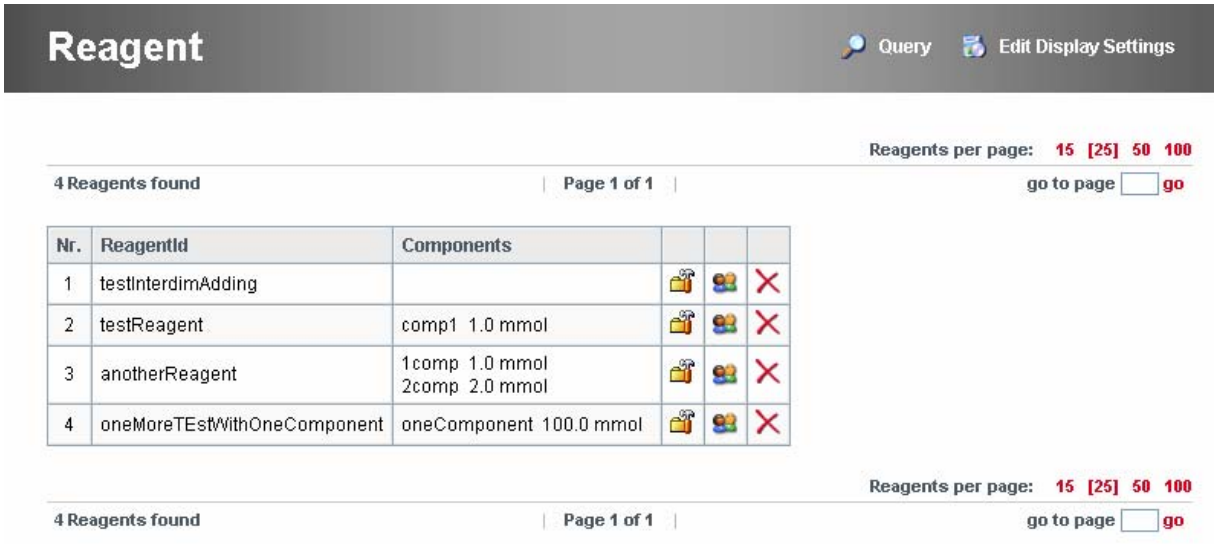
4.12 Reagent

By clicking Sample Processing->Reagent you reach reagent section.

With the “Add Reagent” you can add reagents.



With a click on the button “Find All Reagents” you get an overview of all your reagents:



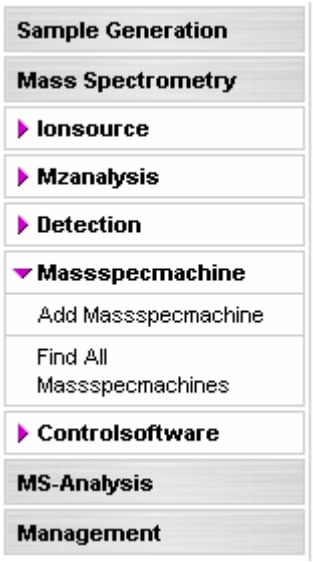
5. Mass Spectrometry:

This section describes machine and software settings for the mass spectrometry experiment.

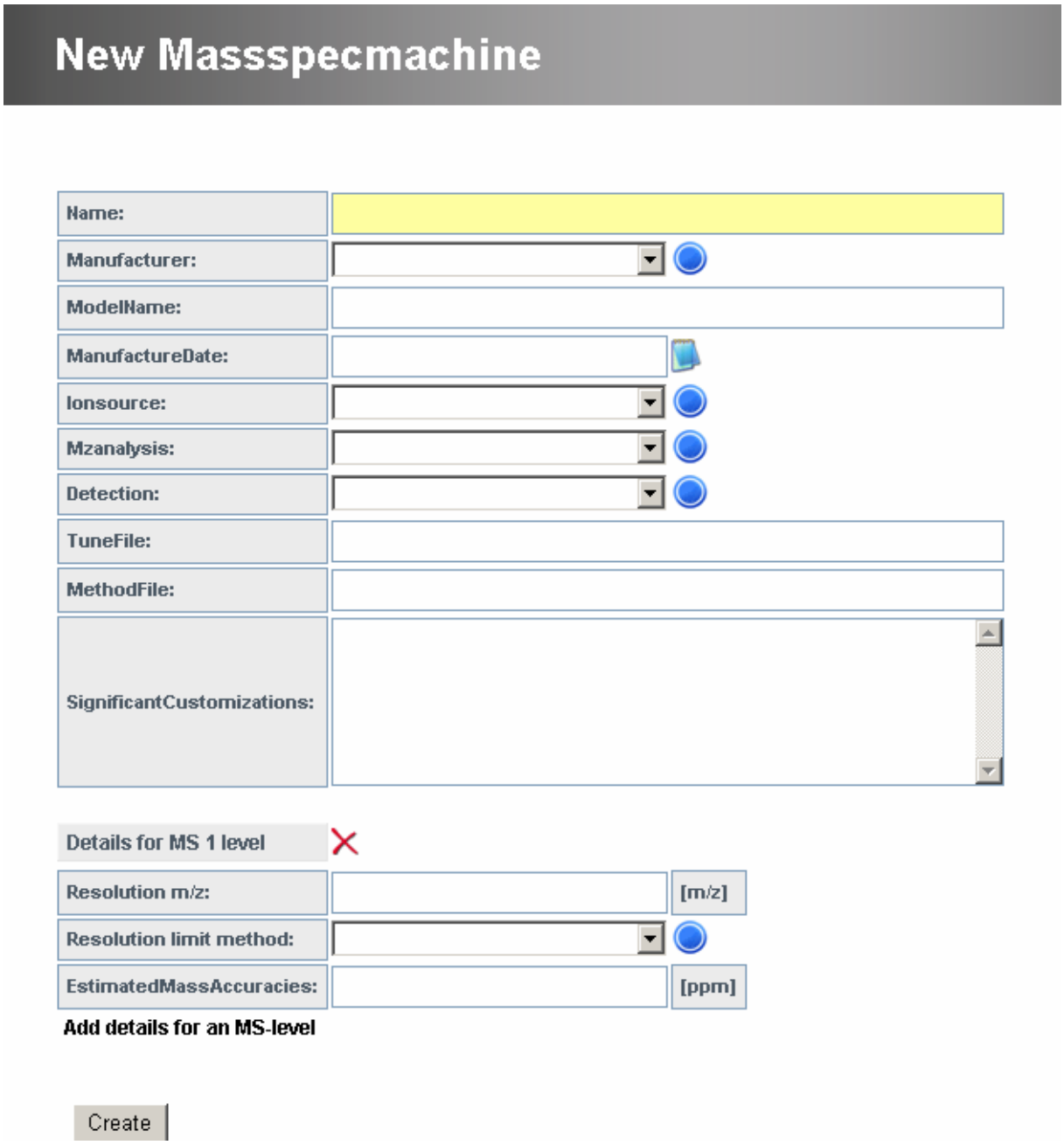
5.1 Mass Spectrometry Machine:

The main part of this section is the mass spectrometry and the other parts (except “Controlsoftware” see chapter 5.5 “Control Software”) are linked to this part. There are two

ways how to reach this part. The first one is by the link in the create/edit page of the mass spectrometry experiment (see chapter 6.1 “Mass spectrometry experiment”), the second one is by clicking on Mass Spectrometry->Massspecmachine.



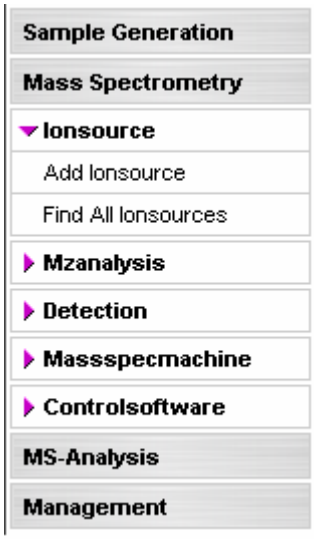
With the “Add Massspecmachine” you can add new mass spectrometry machines.



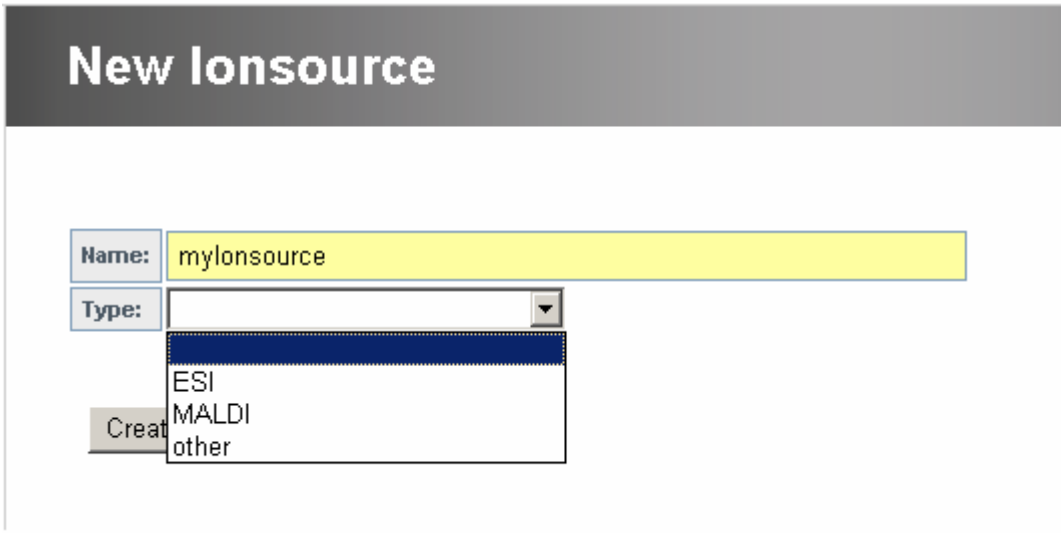
If your desired ionsource,mz analysis or detection is not in the list you can add it directly with the blue button on the right side of the select field. Read more about organisms in chapter 5.2 “Ionsource”, about mz analysis in chapter 5.3 “Mzanalysis” and about detection in chapter 5.4 “Detection”. The links “Add details for an MS-level” add details for each MS-level. You should enter details for all used MS-levels. With a click on the “Find All Massspecmachines” button you get an overview of all your mass spectrometry machines:

5.2 Ionsource:

By clicking Mass Spectrometry->Ionsource you reach the ionsource section.

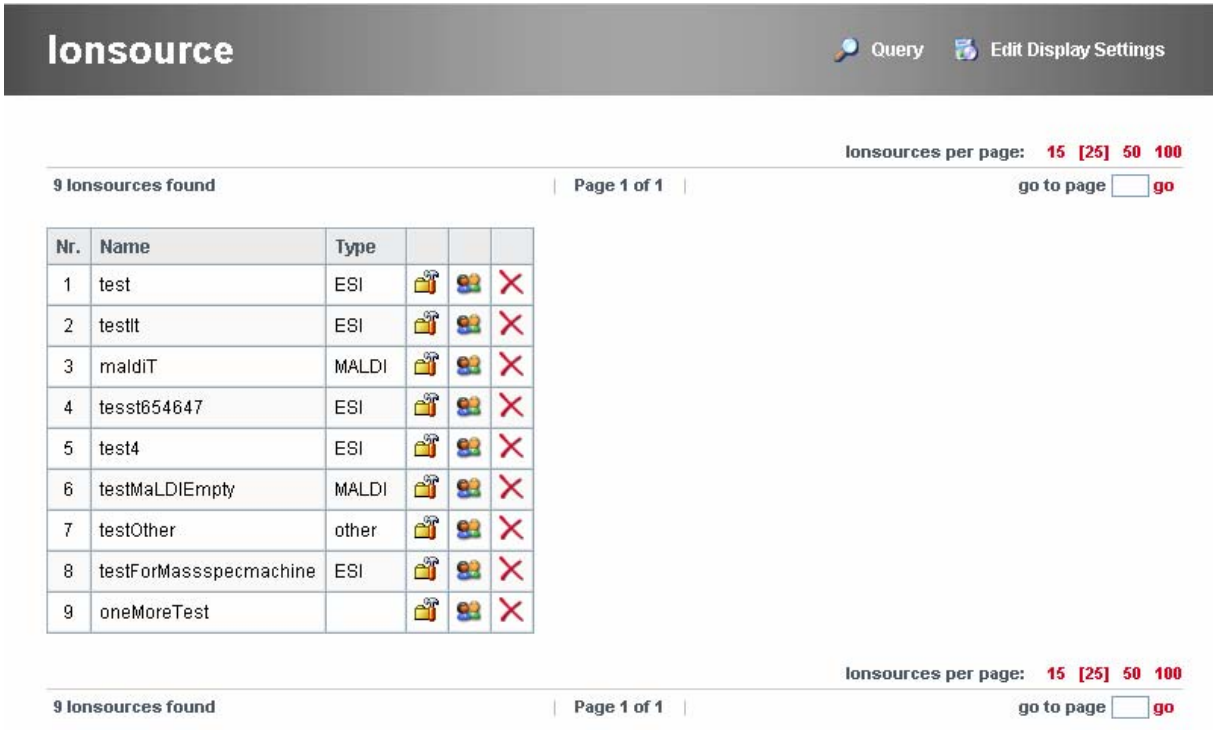


With the “Add Ionsource” you can add new ionsources.



There are 3 types of ionsources (Electrospray chapter 5.2.1, MALDI 5.2.2 and other 5.2.3) available and the input page changes correspondingly.

With a click on the button “Find All Ionsources” you get an overview of all your ionsources:



5.2.1 Electrospray:

New Ionsource

Name:	myTestIonSource
Type:	ESI

Supply

SupplyType:	fed
Cycletime MS1:	[ms]

Add Cycle Time

Solvent

SolventComposition:	
SolventFlorate:	
SolventFlowrateUnits:	

Interface

InterfaceManufacturer	
InterfaceName:	
InterfaceCatalognumber:	
InterfaceDescription:	

Sprayer

SprayTipManufacturer:	
SprayerName:	
SprayerCatalognumber:	
SprayerCoating:	
SprayerDescription:	
SprayTipVoltage:	[V]
SprayTipDiameter:	
ConeVoltage:	[V]

Acceleration and Dissociation

Acclerationvoltage MS1:	[V]

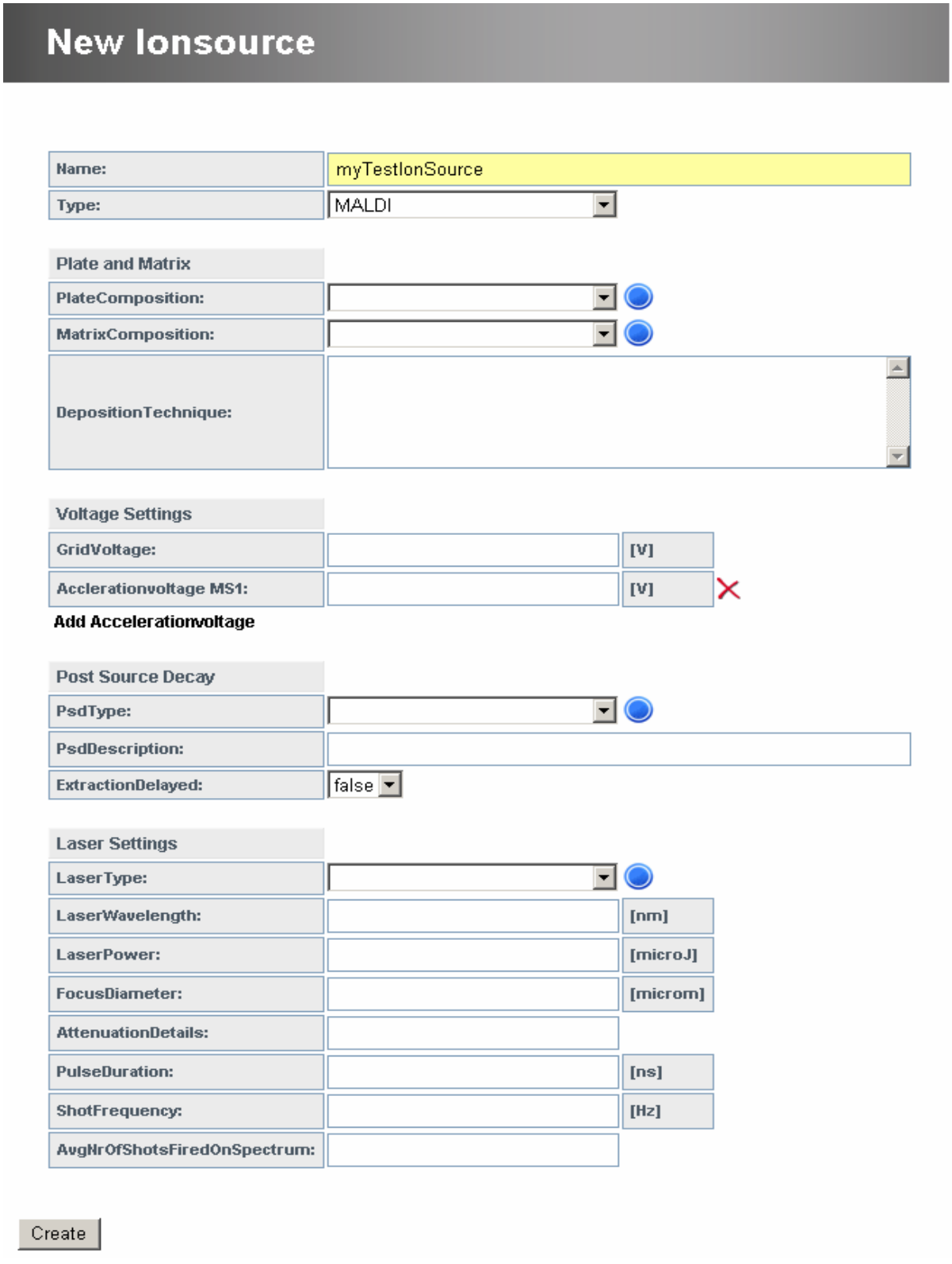
Add Accelerationvoltage

InSourceDissociation:	false
NebulisingGas:	
NebulisingGasPressure:	[bar]

Create

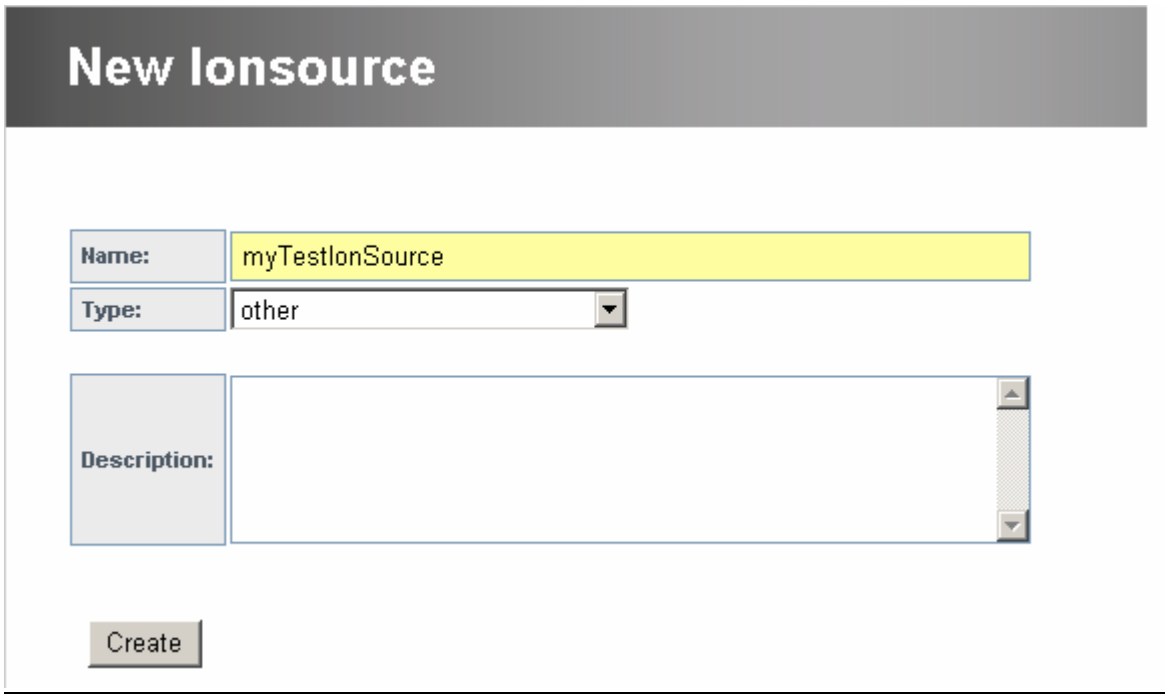
When you change the type to “ESI”, you get the electro spray input form. When you change the “SupplyType” to “fed” then the link “Add Cycle Time” appears and you can enter cycle times for all your MS-levels. In the section “Aceleration and Dissociation” there exists a second link “Add Accelerationvoltage”, where you can enter the acceleration voltages for each MS-level.

5.2.2 MALDI:



When you change the type to “MALDI” then you get the MALDI input page. Use the link “Add Accelerationvoltage” to enter the acceleration voltages for each MS-level.

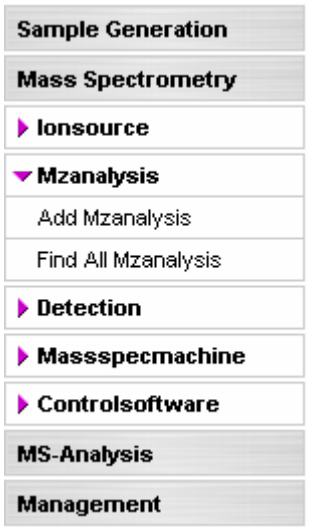
5.2.3 other:



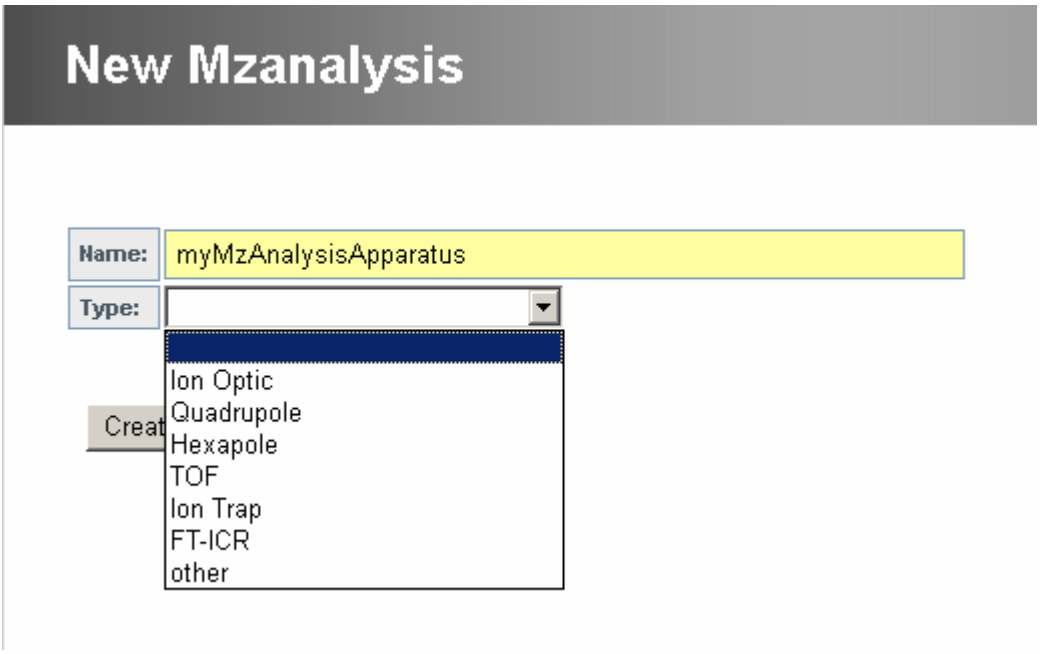
When you change the type to “other” then you get the other ionization input page. There is only an input field for the description of other ionization techniques.

5.3 Mzanalysis:

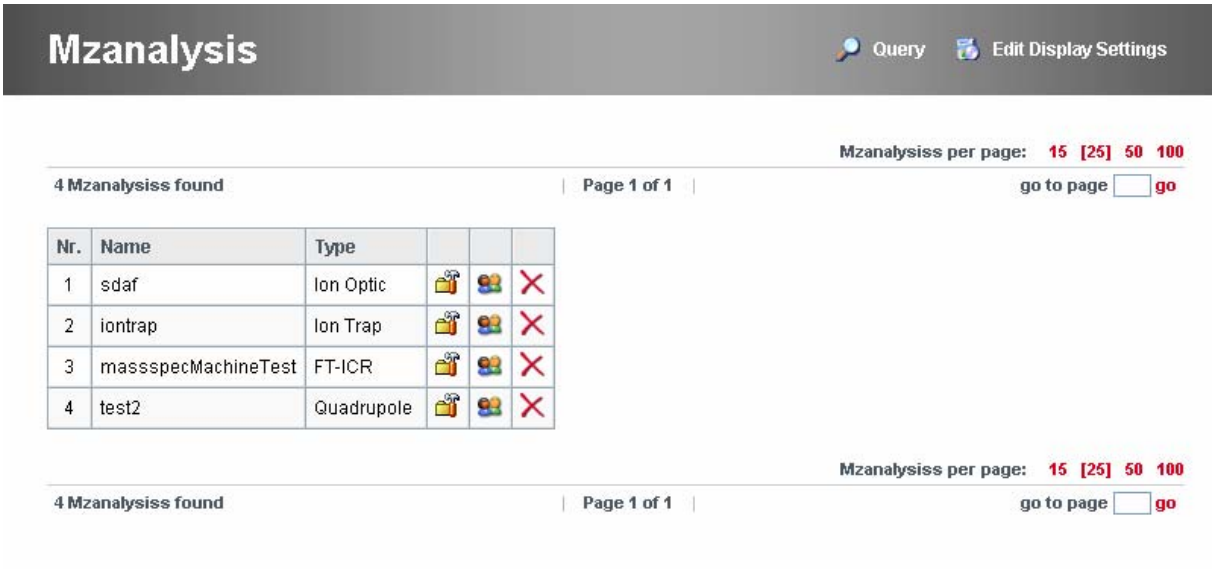
By clicking Mass Spectrometry->Mzanalyisis you reach the mzanalysis section.



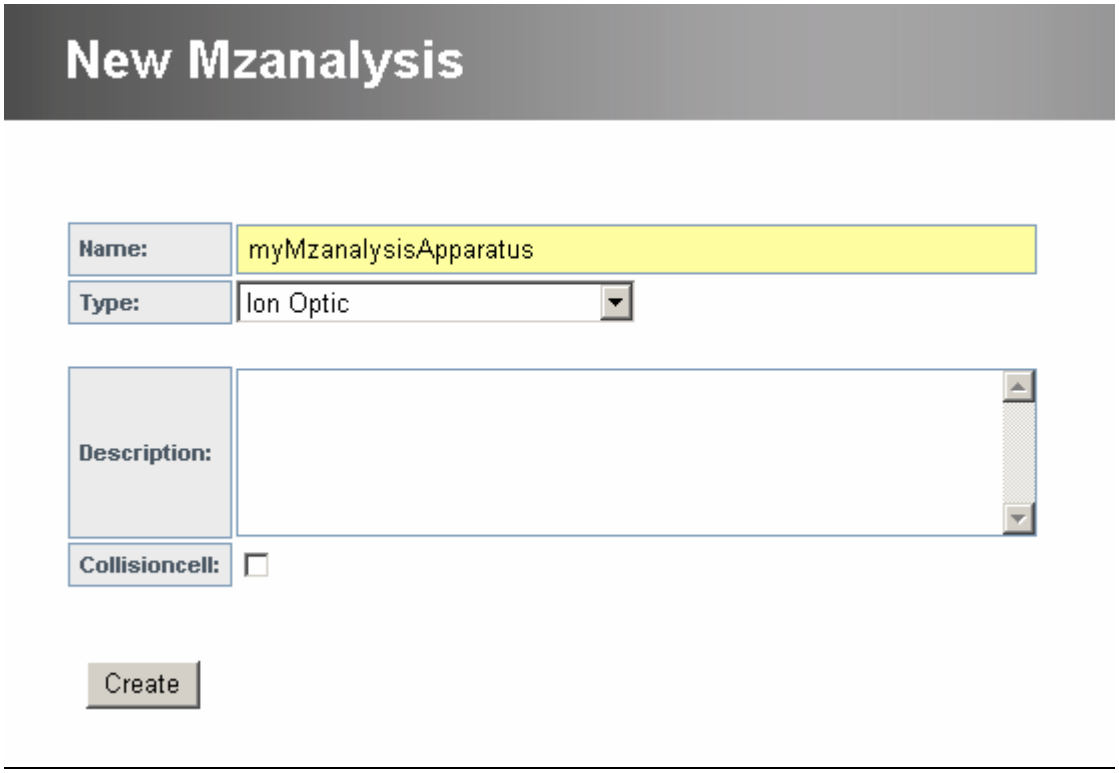
With the “Add Mzanalysis” you can add new mz analysis apparatus.



There are 7 types of mz analysis apparati (Ion optic chapter 5.3.1, Quadrupole chapter 5.3.2, Hexapole chapter 5.3.3, TOF chapter 5.3.4, Ion Trap chapter 5.3.5, FT-ICR chapter 5.3.6 and other 5.3.7) available and the input page changes correspondingly.
With a click on the button “Find All Mzanalysis” you get an overview of all your mz analysis apparati:



5.3.1 Ion optic:



For the ion optic only a description field is necessary. All of the mzanalysis types have a check box where you can enter details about the collision cell (see chapter Collision Cell 5.3.8).

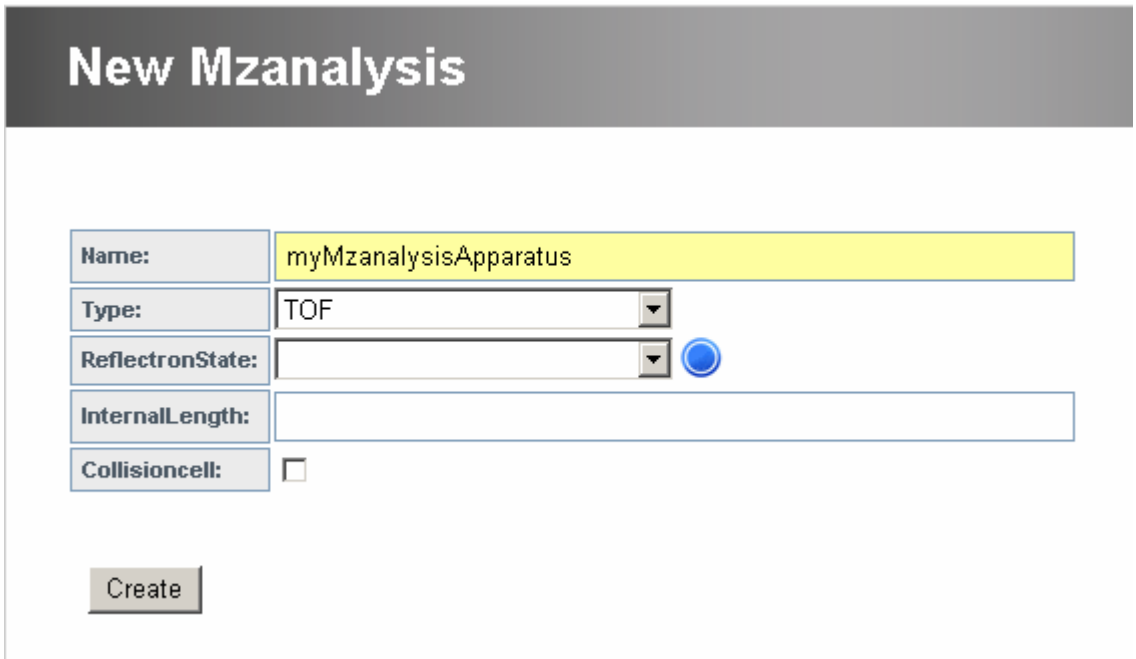
5.3.2 Quadrupole:

Same input page like ion optic see 5.3.1.

5.3.3 Hexapole:

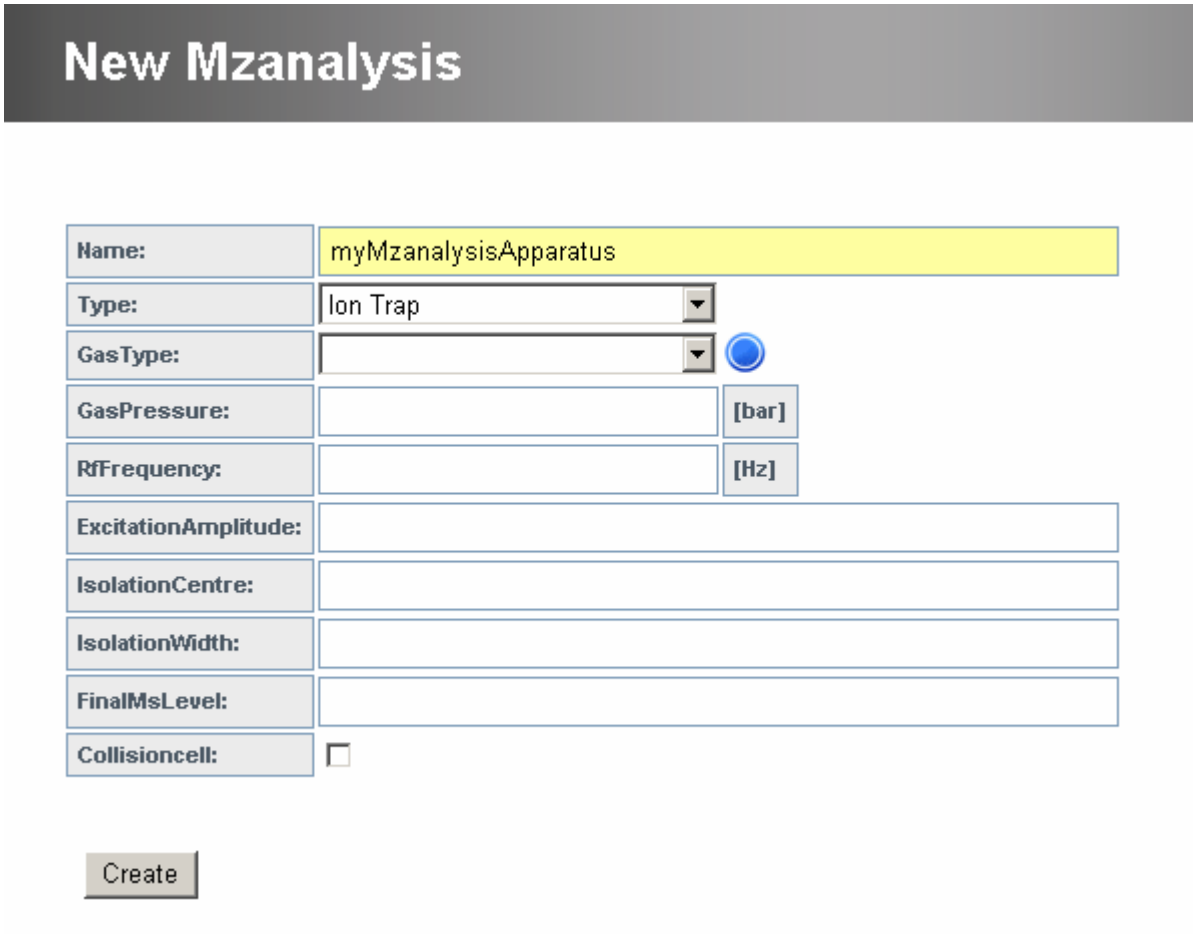
Same input page like ion optic see 5.3.1.

5.3.4 TOF:



All of the mzanalysis types have a check box where you can enter details about the collision cell (see chapter Collision Cell 5.3.8).

5.3.5 Ion Trap:



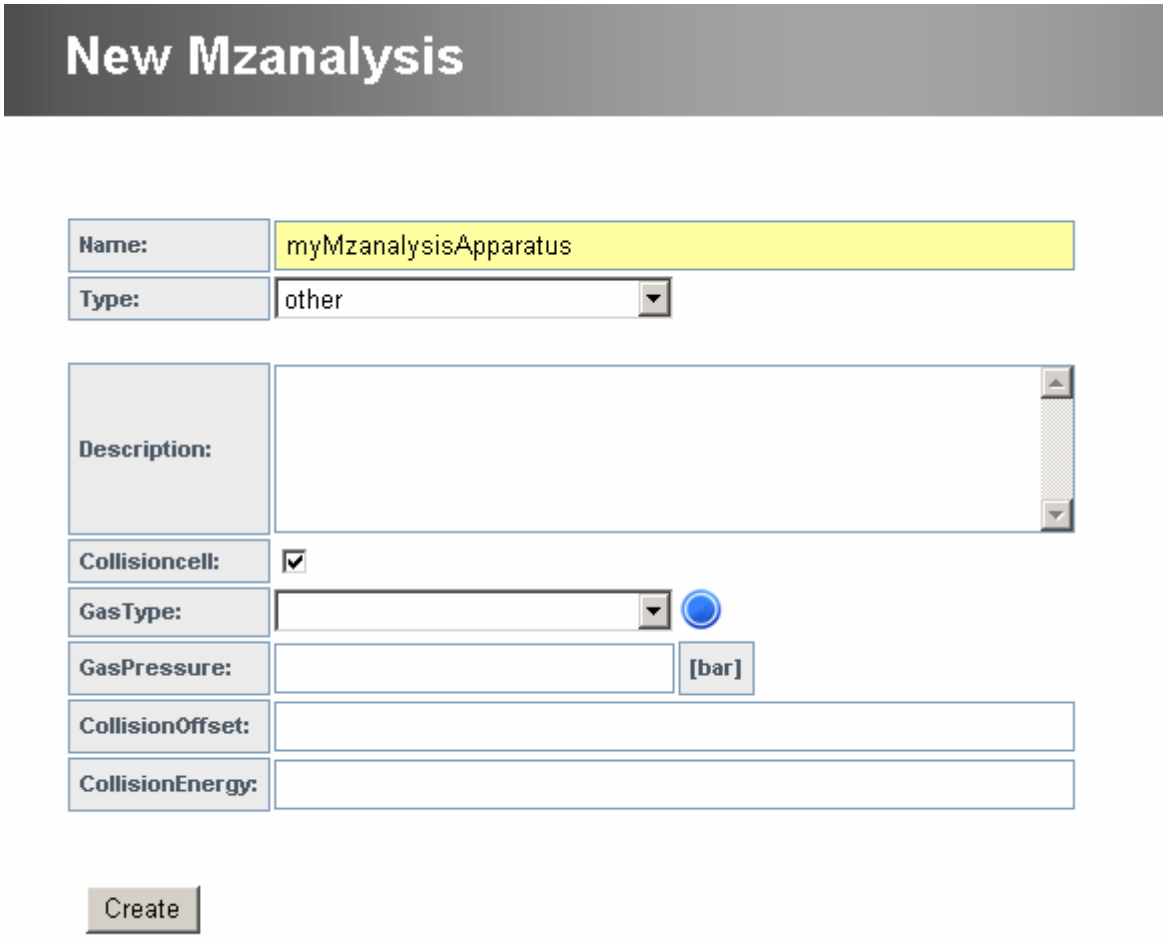
5.3.6 FT-ICR:

Same input page like ion trap see 5.3.5.

5.3.7 Other:

Same input page like ion optic see 5.3.1.

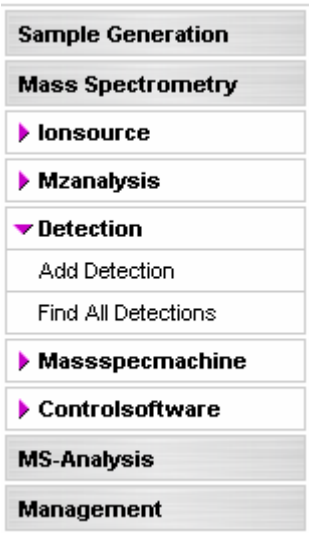
5.3.8 Collision Cell:



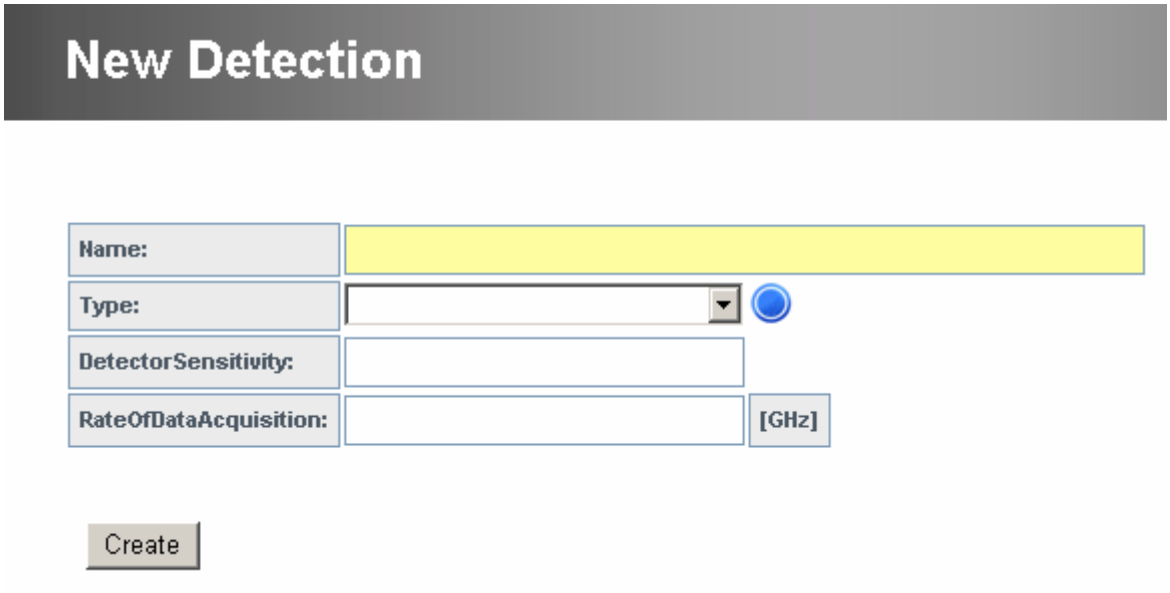
When you check the “Collision cell” check box you can enter information about the collision cell.

5.4 Detection:

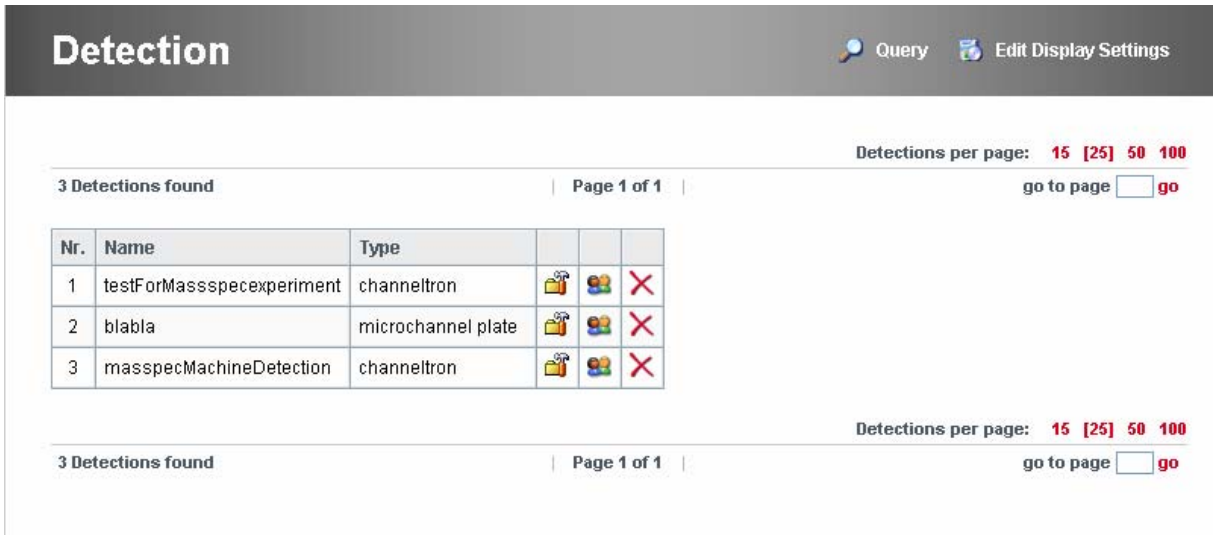
By clicking Mass Spectrometry->Detection you reach the detection section.



With the “Add Detection” you can add a new detector.

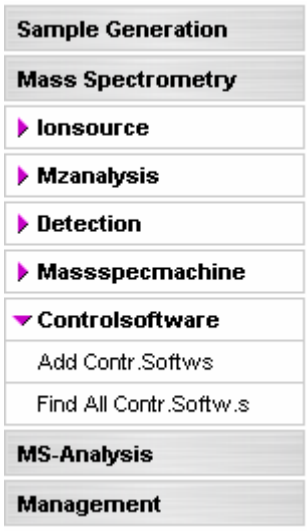


With a click on the button “Find All Detection” you get an overview of all your detectors:

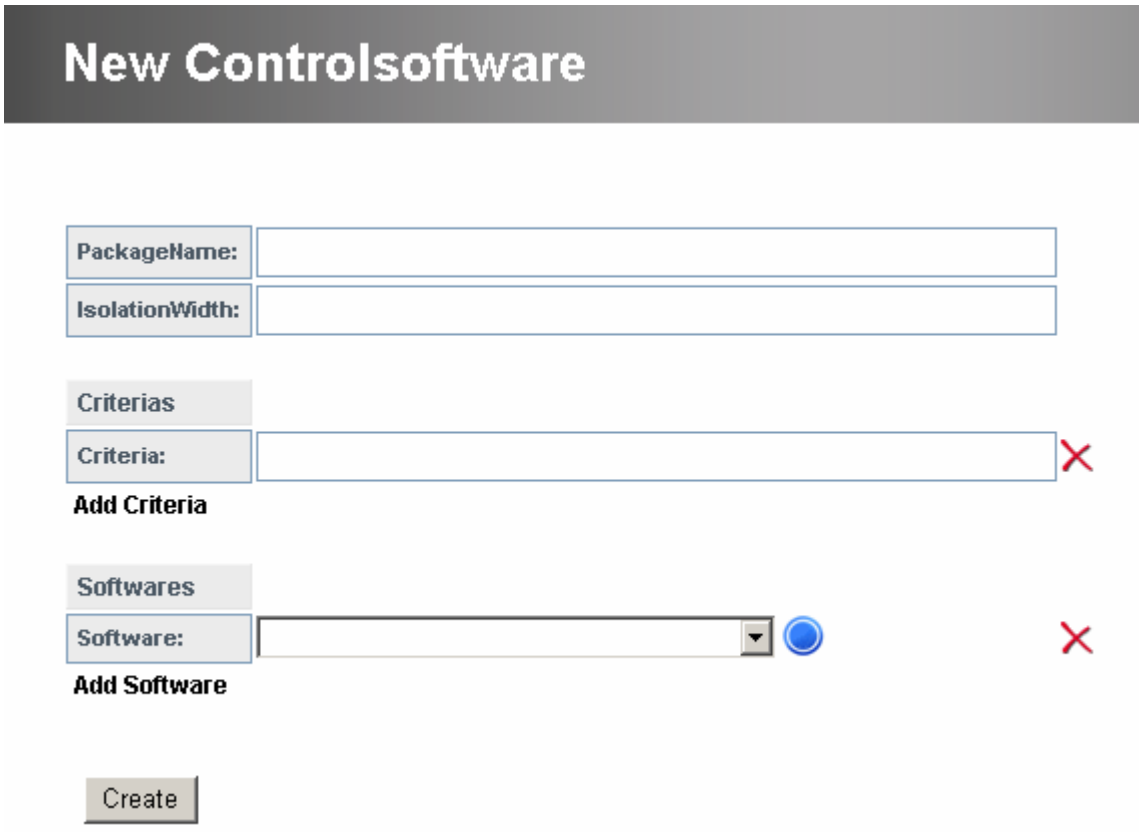


5.5 Control Software:

The control software is needed for mass spectrometry experiments (see chapter 6.1 “Mass spectrometry experiment”). By clicking Mass Spectrometry->Controlsoftware you reach the control software section.

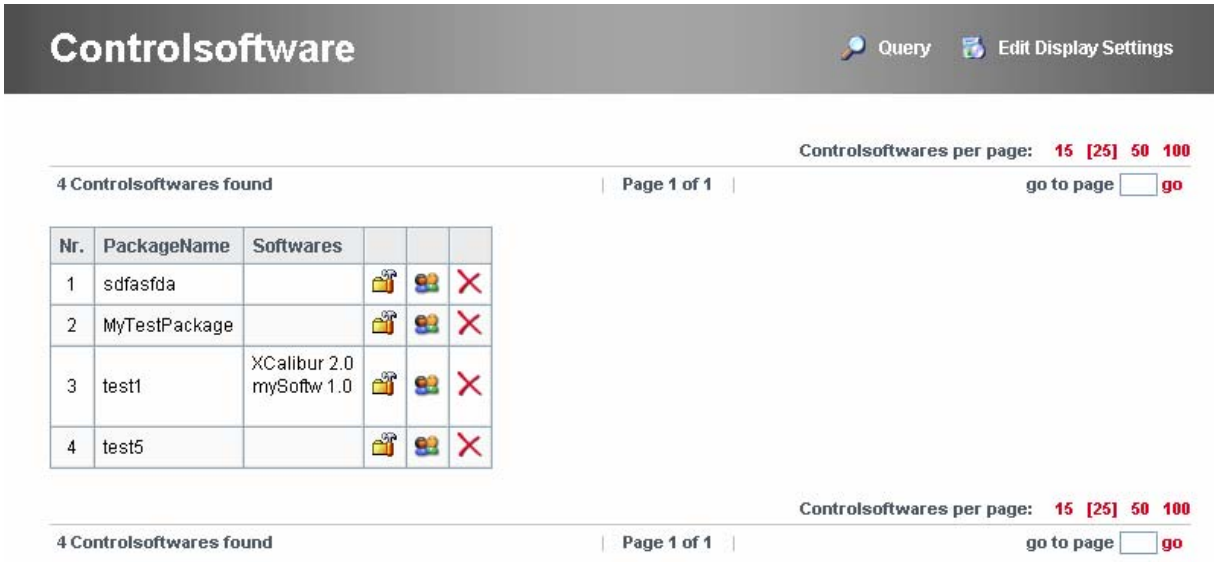


With the “Add Contr.Softws” you can add new control software.



With the link “Add Criteria” you can add switching criteria. With the link “Add Software” you can add software, which the control software consists of. If your software is not in the selection list you can add it with the blue button and you come to the create software page (see chapter 2.4 “Software”).

With a click on the button “Find All Contr.Softw.s” you get an overview of all your control software:

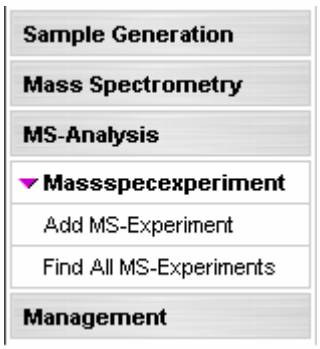


6. Mass Spec Experiment and File Uploading:

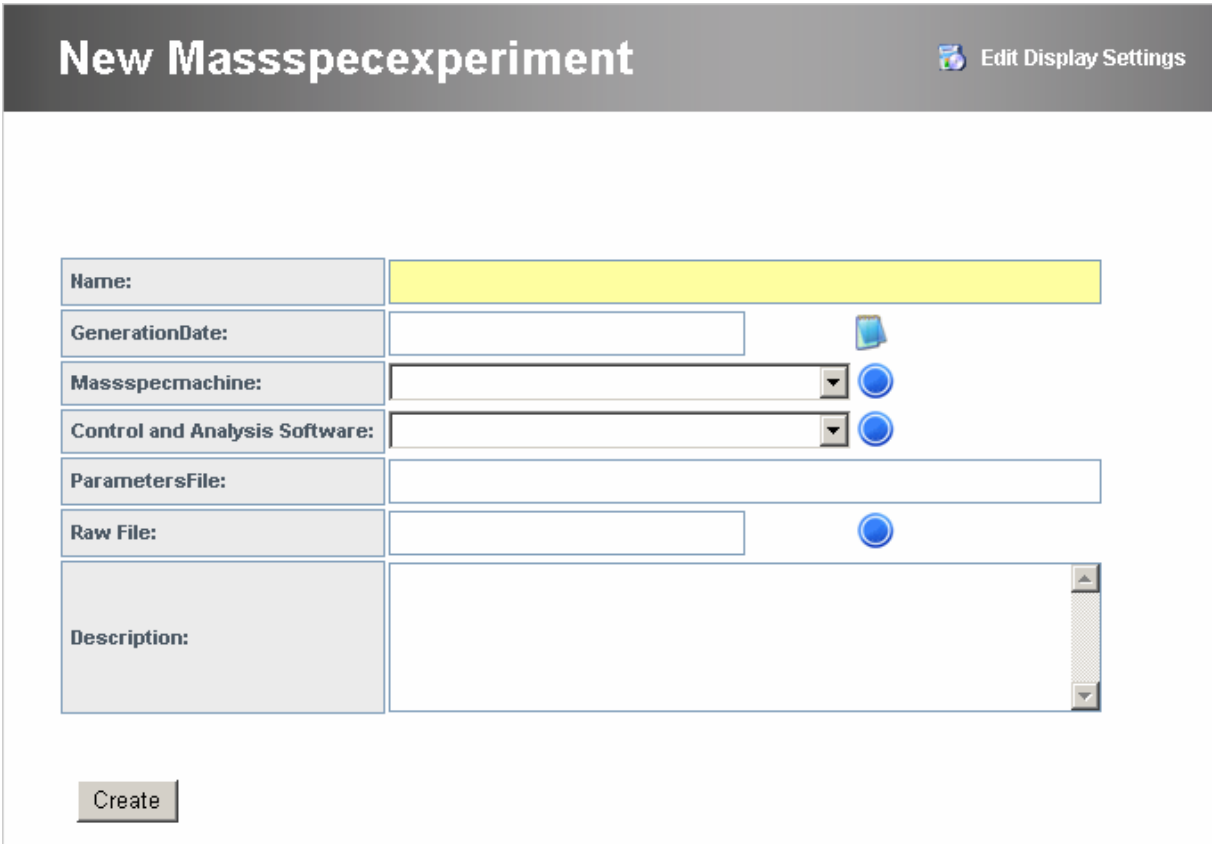
This section describes the generation of mass spectrometry experiments and how you can add searches from different search engines to them.

6.1 Mass spectrometry experiment:

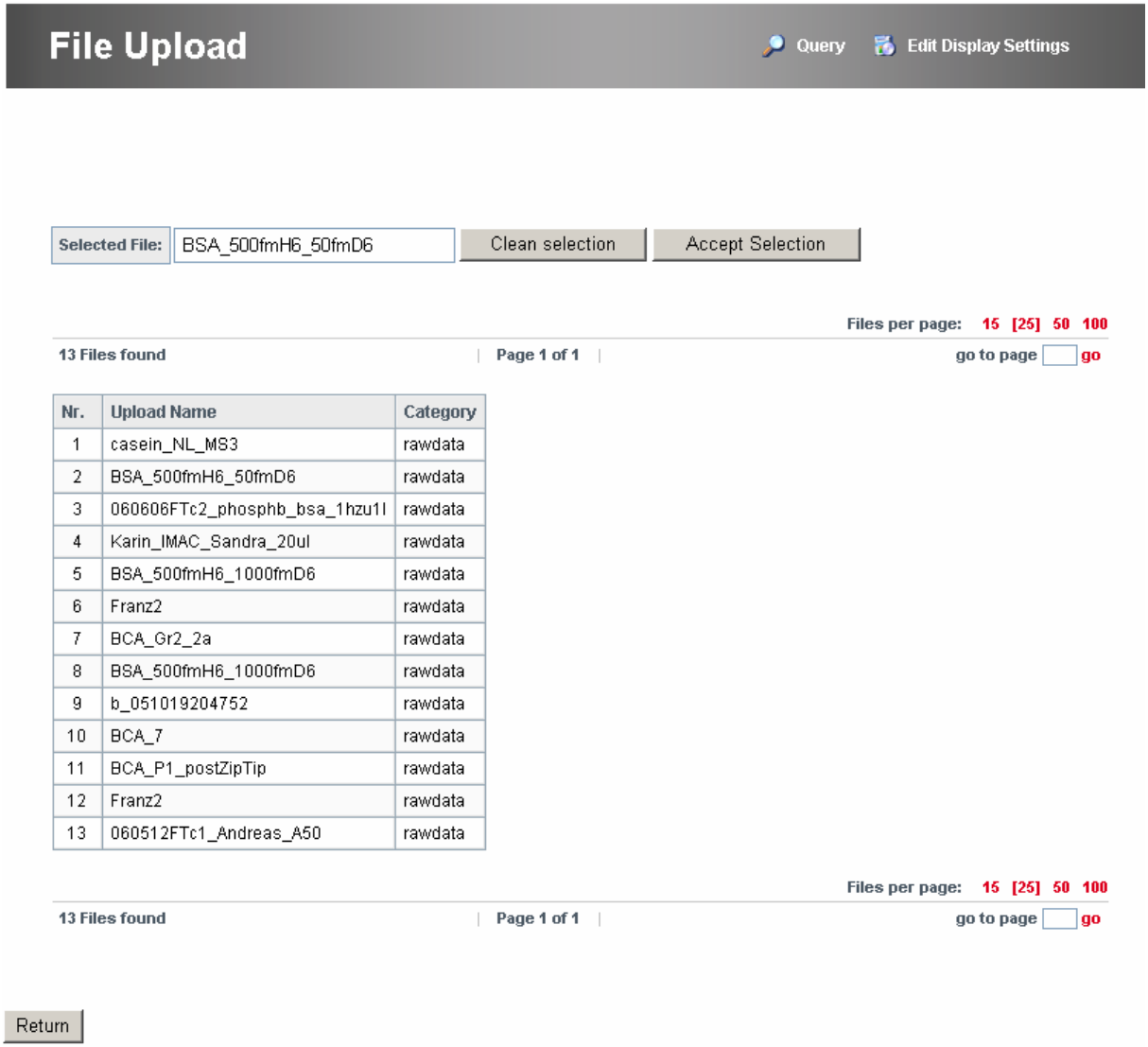
By clicking MS-Analysis->Massspecexperiment you reach the mass spectrometry experiment section. This is a central point, where all the information is linked to one another.



With the “Add MS-Experiment” you can add new mass spectrometry experiment.

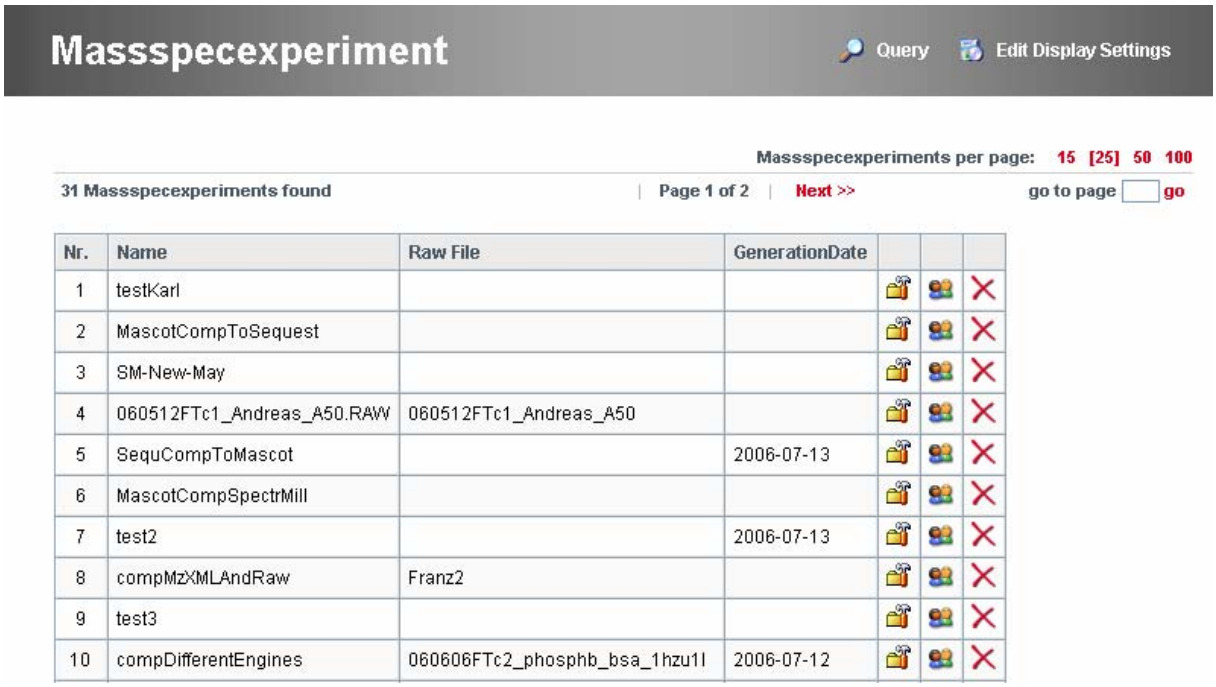


If the desired mass spectrometry machine is not in the select box you can click the blue button on the right side of the select box and you will reach the create page of the mass spectrometry machine (see chapter 5.1 “Mass Spectrometry Machine”). If the desired control and analysis software is not in the select box, click the blue button on the right side of the select box and you will reach the create page of the control software (see chapter 5.5 “Control Software”). To select a raw File click the blue button next to the “Raw File” input field. The following page will appear:



A list of all the raw files uploaded appears. When you click any of the “Upload Names” in the list the name will appear in “Selected File” field. With “Clean selection” you can clean the entry again. With “Accept Selection” this raw file is accepted for that mass spectrometry experiment and will be used for quantitative evaluations, and you return to the create page of the mass spectrometry experiment. If you want to add your mass spectrometry experiment to an analyte, see chapter 4.7 “Adding of Massspec experiments”.

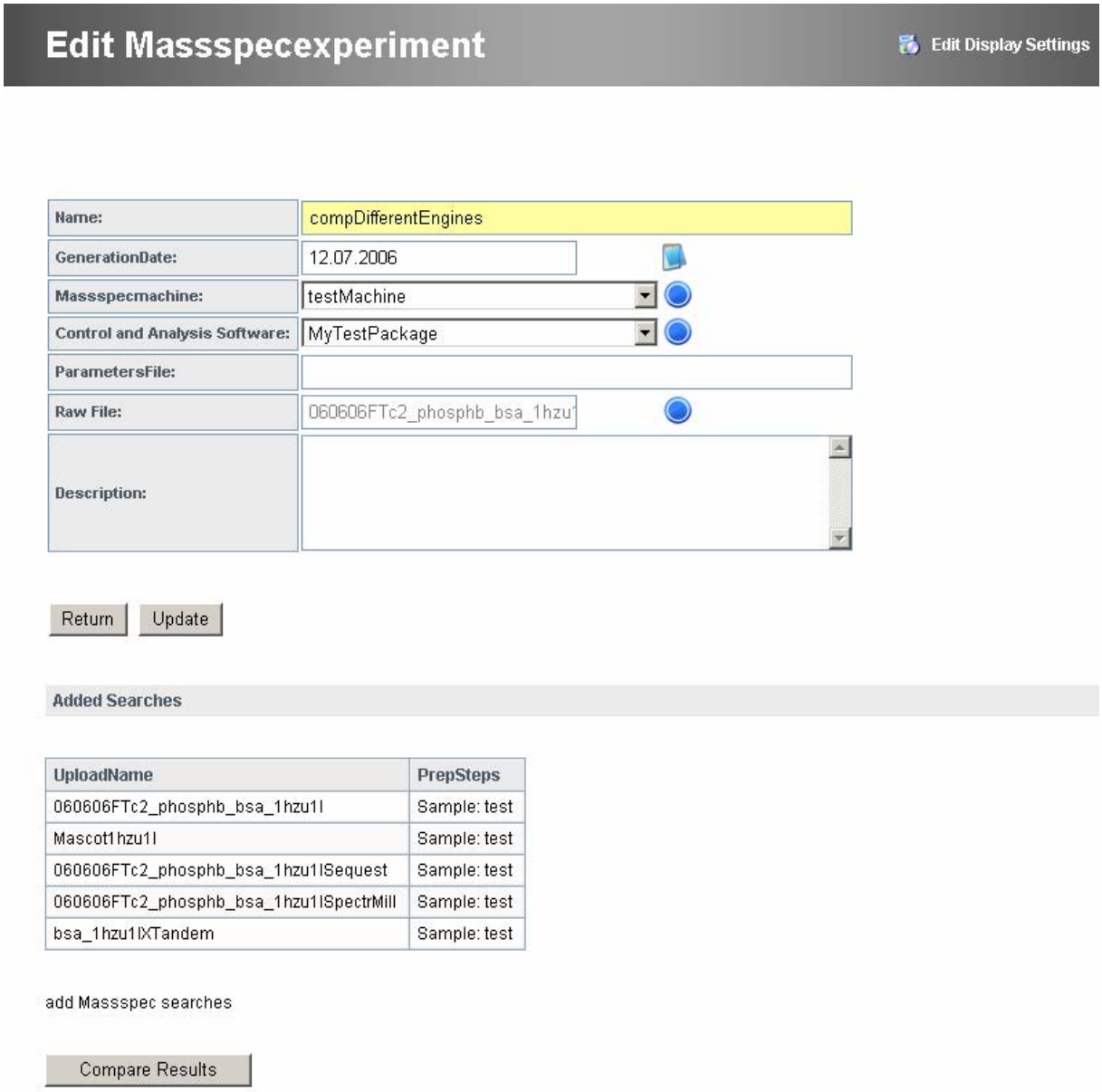
With a click on the button “Find All MS-Experiments” you get an overview of all your mass spectrometry experiments:



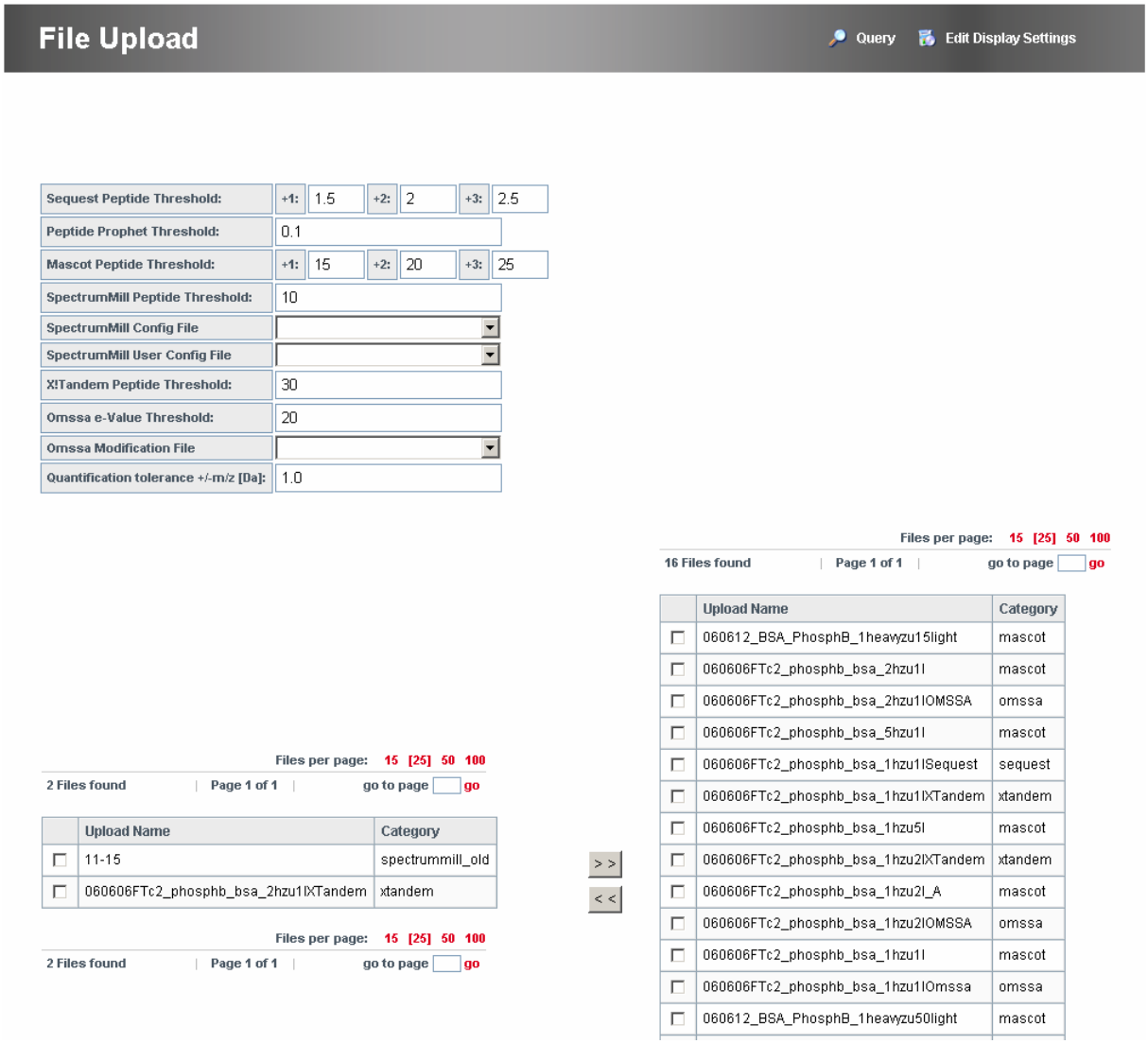
Nr.	Name	Raw File	GenerationDate			
1	testKarl					
2	MascotCompToSequest					
3	SM-New-May					
4	060512FTc1_Andreas_A50.RAW	060512FTc1_Andreas_A50				
5	SequCompToMascot		2006-07-13			
6	MascotCompSpectrMill					
7	test2		2006-07-13			
8	compMzXMLAndRaw	Franz2				
9	test3					
10	compDifferentEngines	060606FTc2_phosphb_bsa_1hzu1l	2006-07-12			

6.2 File parsing into MASPECTRAS:

When you click on the name of the mass spectrometry experiment or the edit button, you will get the following view of your mass spectrometry experiment:



When you follow the link “add Massspec searches”, you will get a page where you can upload you search results from Sequest, Mascot, Spectrum Mill, X! Tandem, or OMSSA.



The thresholds are necessary to remove the most unlikely data. The peptide prophet threshold affects Sequest and Mascot only. For SpectrumMill (new version) you have to specify your Spectrum Mill Config File (smconfig.xml) and if you have added modificitations also the Spectrum Mill User Config File (smconfig.custom.xml). For OMSSA you have to specify the Omssa Modifications File (mods.xml).

Adding and removing of searches to a spot (or band) works the same way like adding of samples to experiments works (see section 3.2.2).

After the files have been selected the following processes are started (you will see the same steps in the Upload Status Section):

“Step 1/5 (Parsing)”: Reads the necessary file (or files), filters the data and builds the corresponding value objects
“Step 2/5 (Transferring hits)”: Stores the found proteins into the database
“Step 3/5 (Storing peaklists)”: Stores the peaklists and the connected peptidehits and links them to the corresponding proteins

"Step 4/5 (Calculating)": Retrieves the protein sequences from the database (if not already stored), calculates the proteinhit score and the sequence coverage of the hit

"Step 5/5 (Protein Grouping)": Clusters similar proteins together in protein groups.

After these five steps an automatic calculation of a relative quantity for each peptide is started, when a raw file for the mass spectrometry experiment is selected (see chapter 6.1 "Mass Spectrometry Experiment"). The progress bar for the calculation starts again at 0%. You can meanwhile validate your data. The view on the data is the same, the only difference is that in the peak-area file you will find no value until the calculation has finished.

7. Analysis:

There are two ways to analyse (compare) your data:

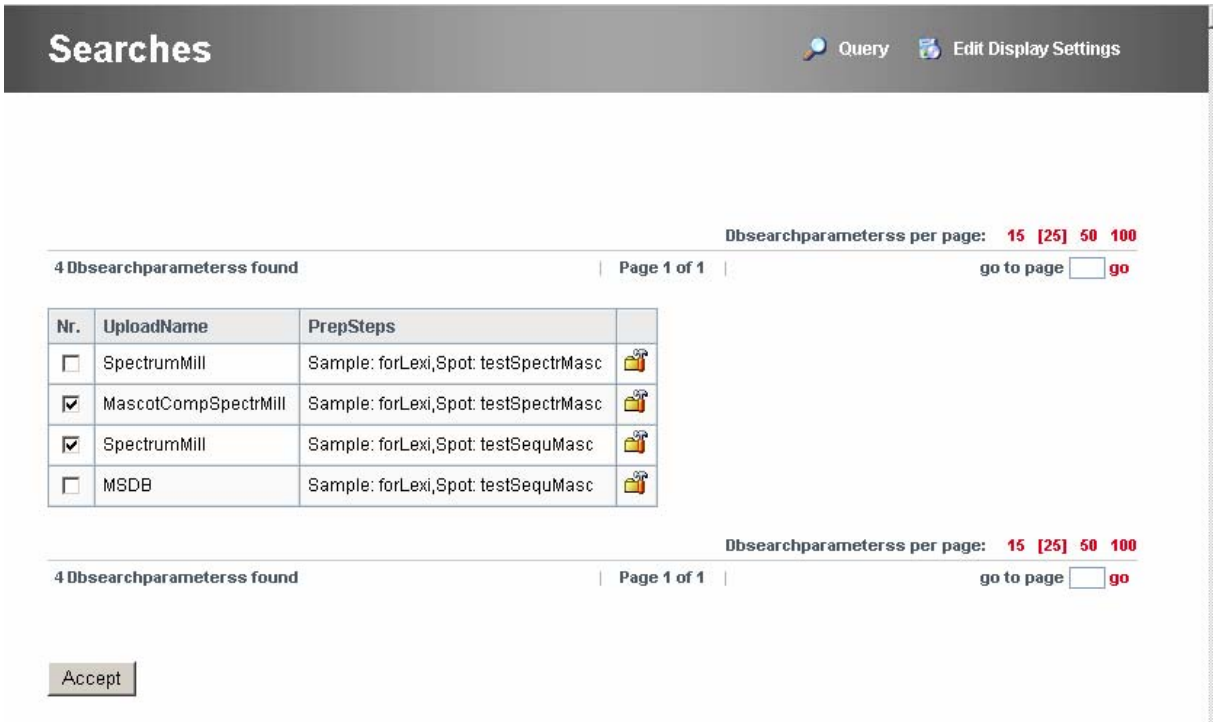
1. To click directly on the upload name table below the mass spectrometry experiment (see first picture section 6.2 "File parsing into MASPECTRAS")
2. To use the

   button.

You will find this button when you list your samples from one experiment (then you can compare all searches that are in this experiment) or in a list of the "Uploaded Searches" in the mass spectrometry experiment (see first picture section 6.2 "File parsing into MASPECTRAS). Further buttons of that type are planned at every analyte and at every sample processing step.

When you push this button you can select which of the uploaded searches you want to compare. All uploaded searches below this data point are displayed. Also the preparation steps that have been used are shown.

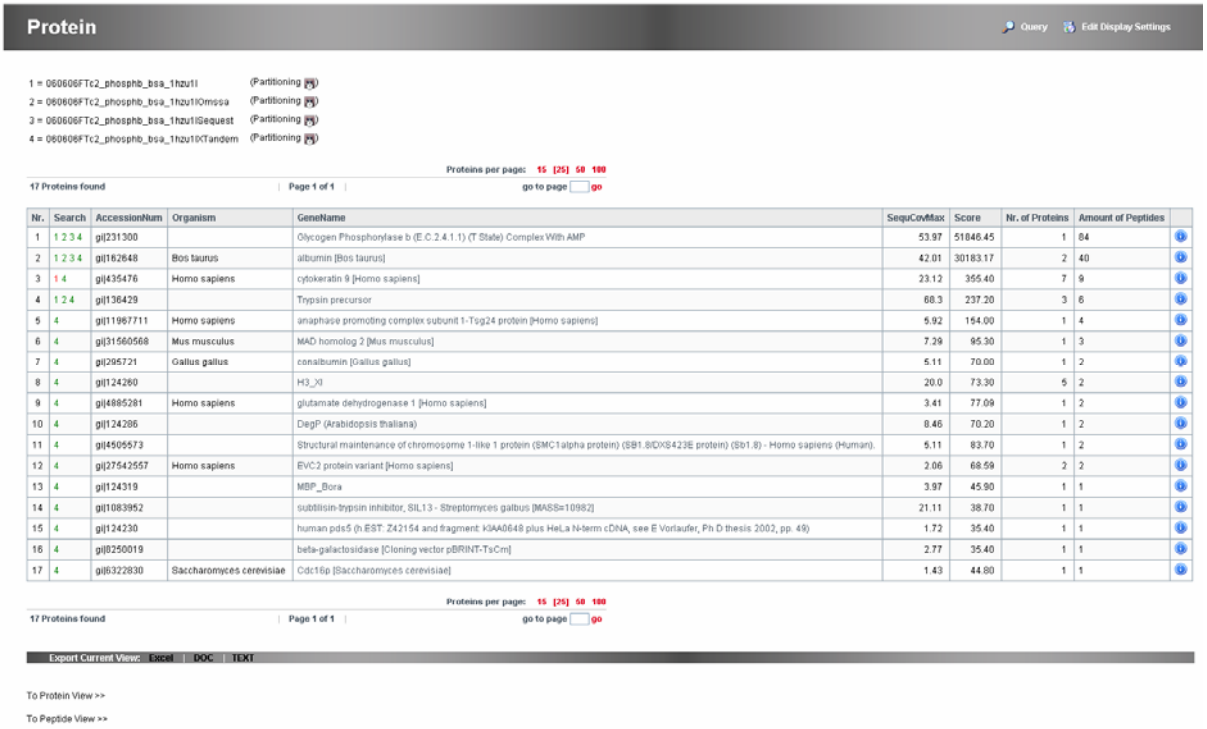


When you click the , you can edit the mass values of your uploaded modifications. This could be useful for the comparison, because the system could only group together peptides with the same mass shift.

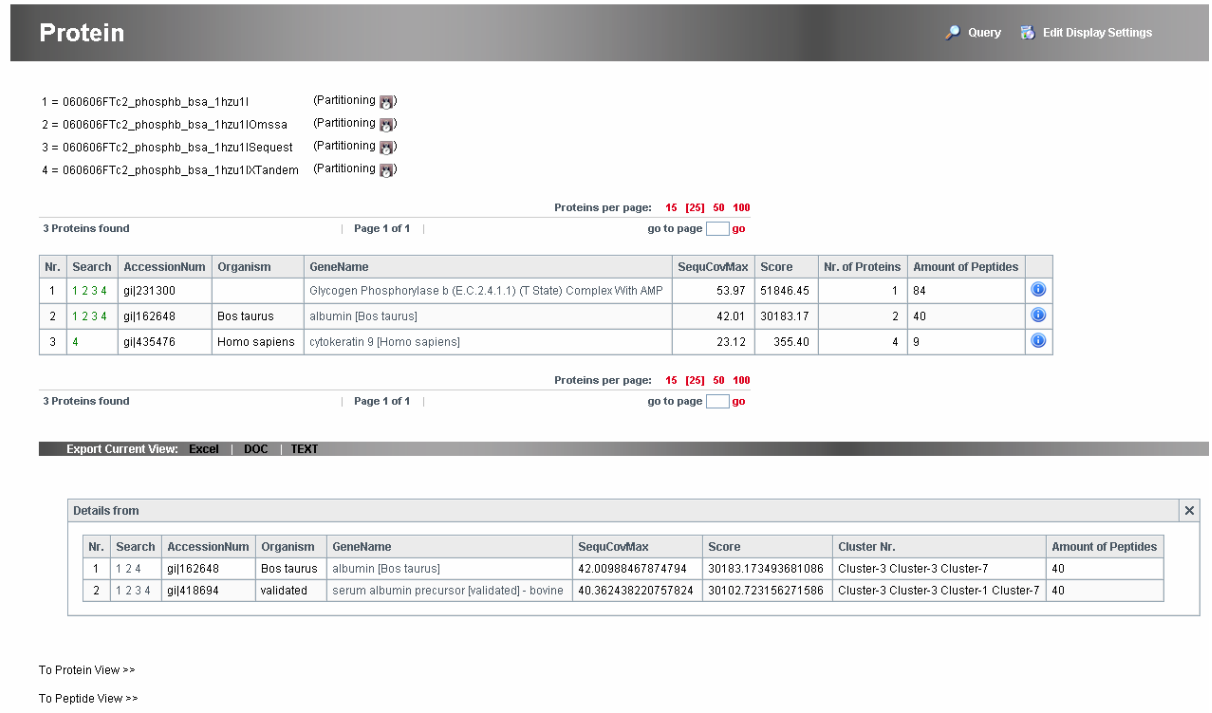
Hydrogen	1.007825
Carbon	12.0
Nitrogen	14.00307
Oxygen	15.99491
Electron	5.49E-4
C_term	17.002735
N_term	1.007825
Oxidation (M)	15.994904
NeutralLoss1	0.0
Phospho (ST)	79.966324
NeutralLoss2	97.976896
Phospho (Y)	79.966324
NeutralLoss3	0.0

Return Update

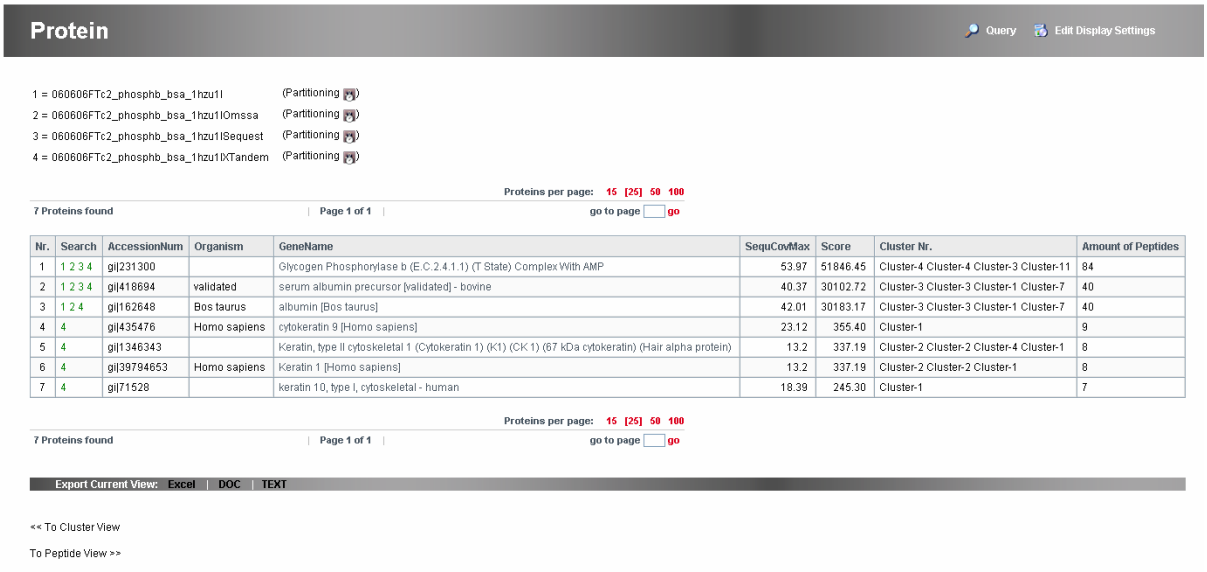
7.1 Protein comparison:



Below the header the searches that you have selected are listed by their names and numbers are assigned to find them in the table below. Next to the names there are links in brackets called “Partitioning”. With these links you reach a page with a more detailed description of the cluster (7.2).
The table below lists the found proteins. When you reach the page the proteins are clustered together. The proteins are sorted by their sequence coverage. The protein with the best sequence coverage is getting displayed as substitute for all the proteins in the cluster. In the “Search” column the numbers indicate the searches, by which a protein has been found. You can reach the combined peptide view of the protein when you click on the “GeneName” of the protein (7.3). If you want to see the peptide view of only one search there is a link on the number if the number is green. A red number indicates that this substitute protein was not found with this search but another protein in the cluster has been found with this search.
The “Nr. of Proteins” column shows you how many proteins have been put together in one cluster. When you push the blue button you get all proteins of that cluster listed.



The “Cluster Nr.” indicates the cluster where the protein is located. The order is the same as in the “Search” column.
If you don’t want to see the clustered view at all you can click on the “To Protein View>>” at the bottom of the page to get all proteins displayed.



The “<< To Cluster View” brings you back the cluster view.

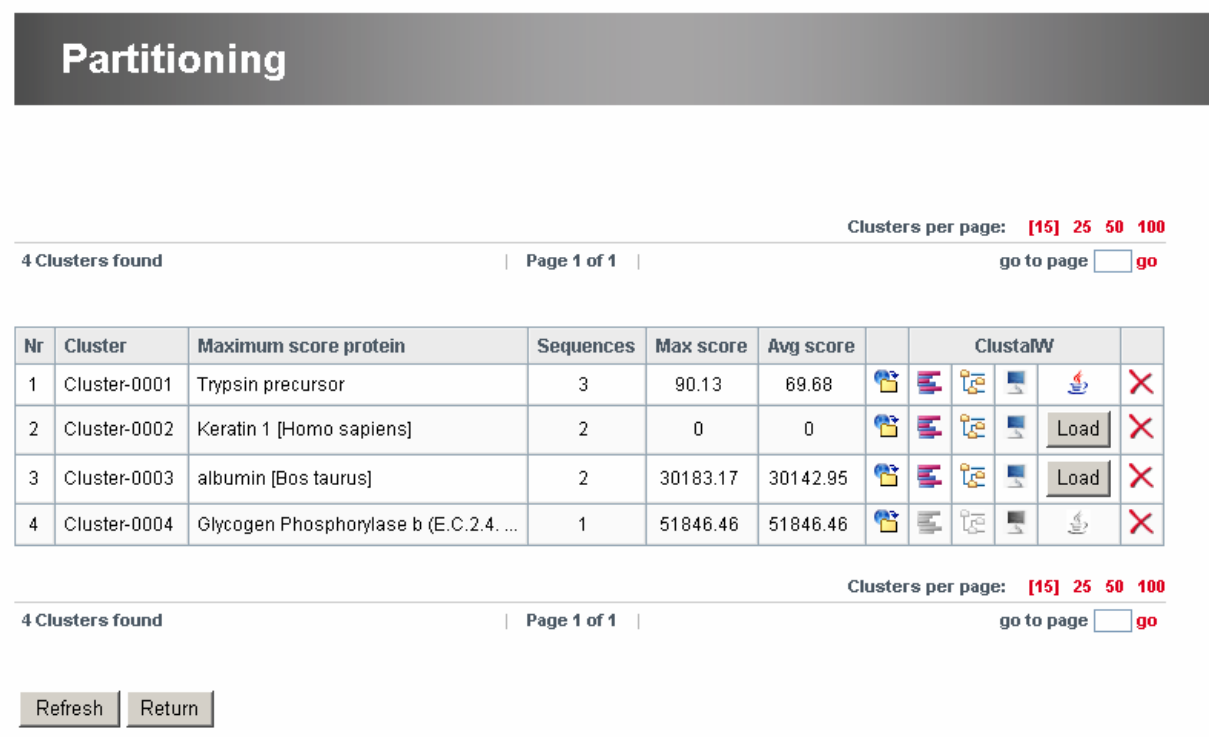
The export bar lets you export the table with the selected columns in different file formats.

The “PRIDE XML” link generates a XML File in the PRIDE 2.0 XML Format, which is needed to export your Experiment to the PRoteomics IDEntifications database, a centralized, standards compliant, public data repository for proteomics data (http://www.ebi.ac.uk/pride/).

To get a valuable XML file be sure that you have entered detailed information about the sample and the massspecmachine including for example the sample origin the masspecmachine analyzers and detectors and the controlsoftware.

The “>> To Peptide View” brings you to the peptide view, where all the peptides of your searches are displayed. It is the same like in 7.3 but the protein sequence is not colored.

7.2 Cluster (Partitioning):



The detailed view of the clusters is reachable by the protein comparisons (7.1). The proteins are sorted by the size of the cluster.

: Download of the involved proteins in FASTA format

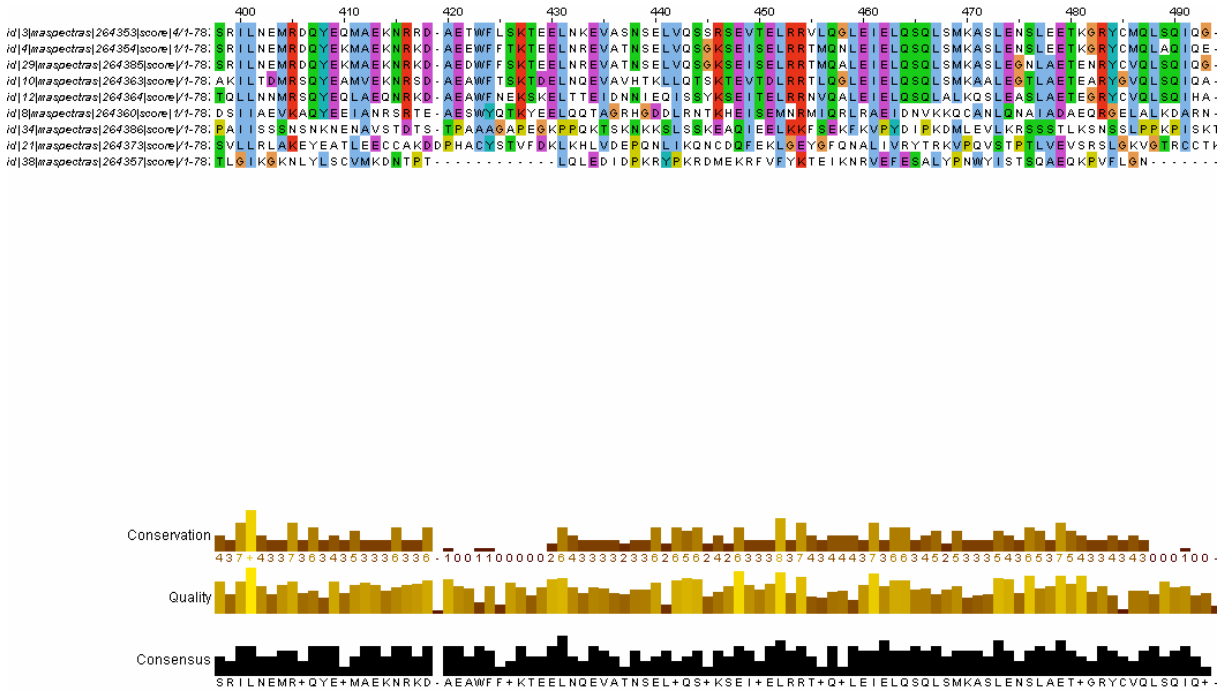
: Download of the alignment of the proteins

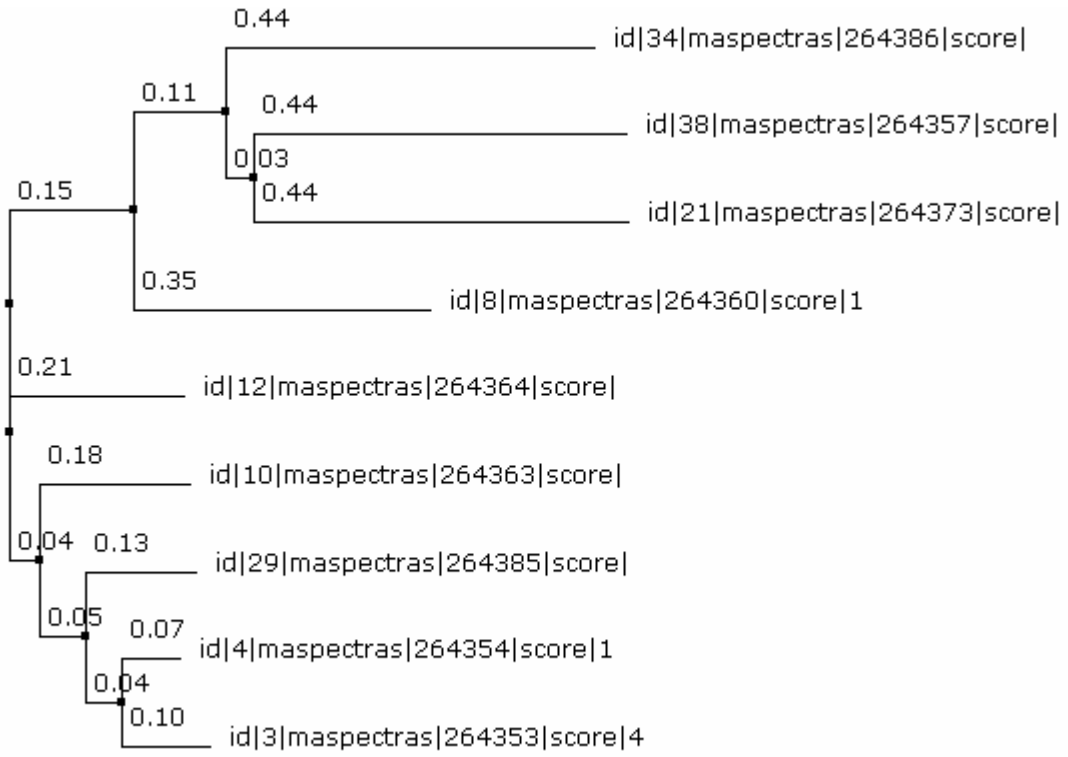
: Download the storage of the tree that you can see in Jalview at the end of this section

: The log-file of the alignment

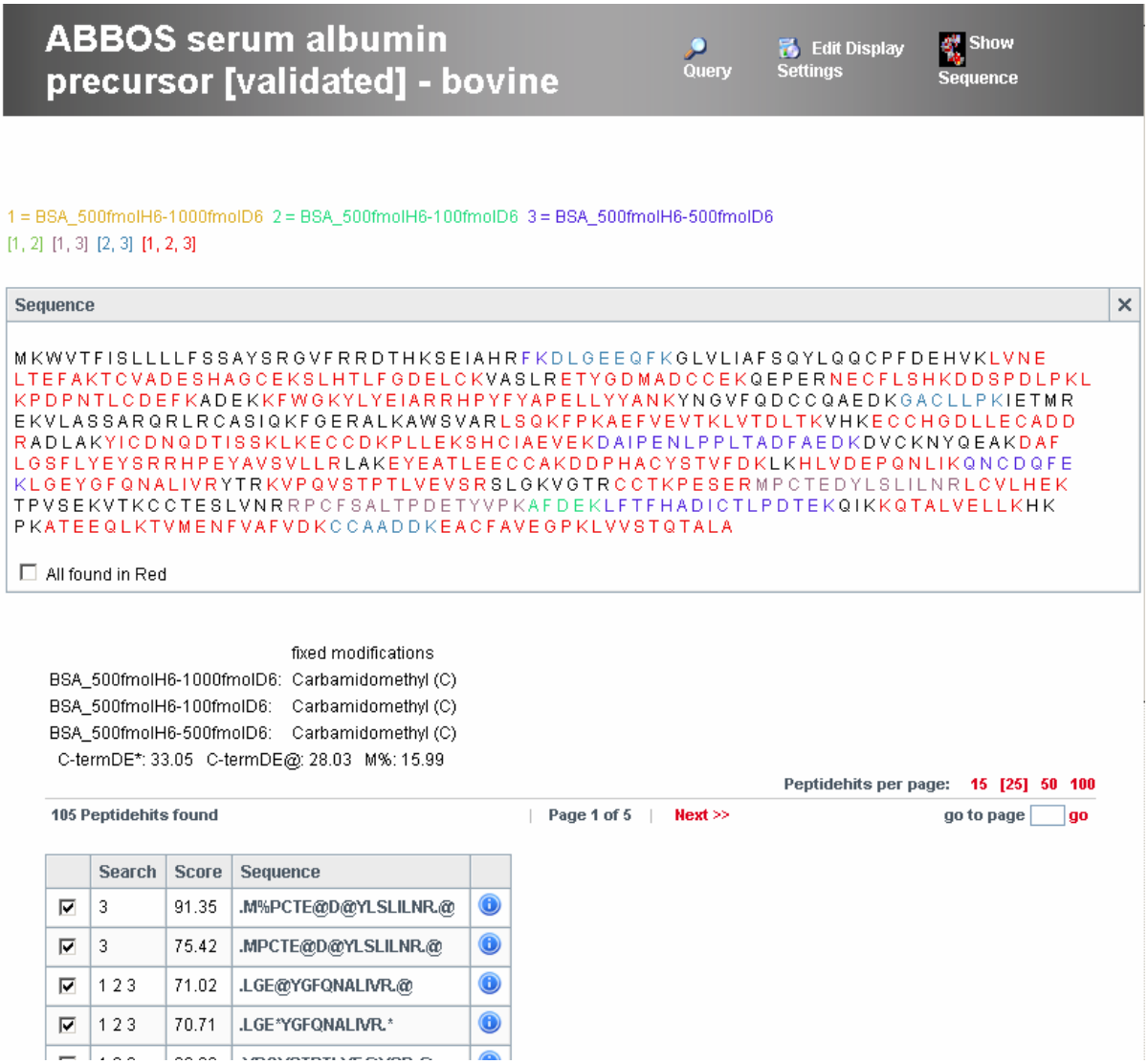
Load : The buttons are Java applets itself and when you want to display a big list all of the buttons all the applets would have to be loaded. As this takes to much time, the Load” button has to be presses to get a corresponding applet.

: Starts Jalview applet to see the alignment


400
410
420
430
440
450
460
470
480
490
id|3|maspectras|264353|score|4/1-78:
id|4|maspectras|264354|score|1/1-78:
id|29|maspectras|264385|score|1/1-78:
id|10|maspectras|264363|score|1/1-78:
id|12|maspectras|264364|score|1/1-78:
id|8|maspectras|264360|score|1/1-78:
id|34|maspectras|264386|score|1/1-78:
id|21|maspectras|264373|score|1/1-78:
id|38|maspectras|264357|score|1/1-78:
Conservation
Quality
Consensus

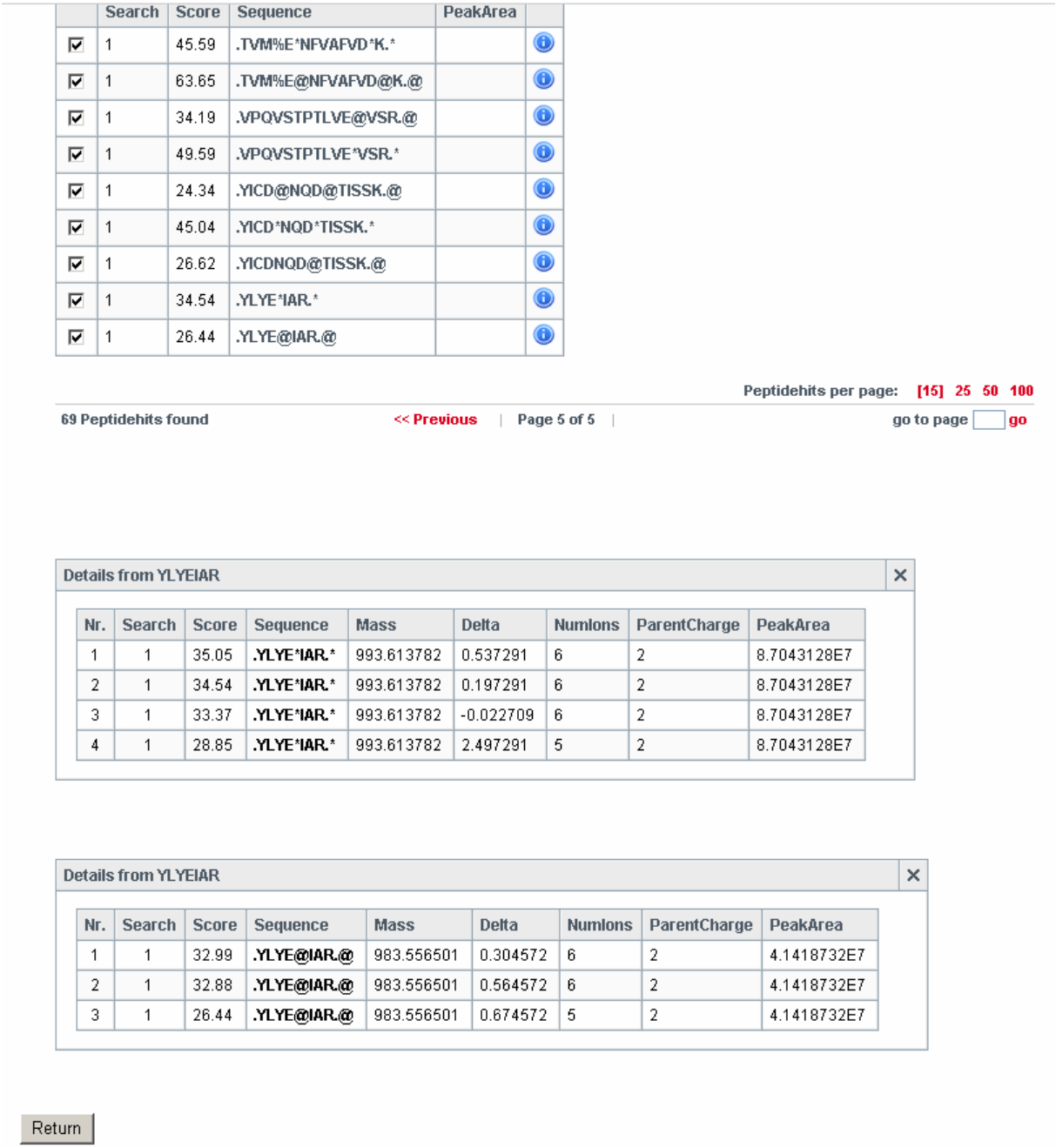

0.44
id|34|maspectras|264386|score|
0.11
0.44
id|38|maspectras|264357|score|
0.03
0.44
id|21|maspectras|264373|score|
0.15
0.35
id|8|maspectras|264360|score|1
0.21
id|12|maspectras|264364|score|
0.18
id|10|maspectras|264363|score|
0.04
0.13
id|29|maspectras|264385|score|
0.05
0.07
id|4|maspectras|264354|score|1
0.04
0.10
id|3|maspectras|264353|score|4

7.3 Peptide comparison:



The gene-name is displayed at the page head. The  button opens the box with the protein sequence again, if you have closed it. Below the page head the searches are listed again. This time dyed in order to recognize them in the protein sequence. Underneath the possible combinations of the searches are colour-encoded as well.
The “Sequence” box has a little checkbox “All found in Red”, which shows all found parts of the sequence in red, if one colour is not easily visible.
Then the searches are listed again and the fixed modifications are given. At the end of the searches the variable modifications are indicated in one row. The affected amino acids are shown followed by the substitute for the modification in the peptide list and the mass shift after the colon.
Below the searches the found peptides are listed, sorted by the score. To indicate by which search the peptide has been found the numbers in the search column are denoted (the same way like in 7.1). If this sequence is a first hit, the sequence is in bold letters. When you uncheck the checkbox in front of a peptide, this peptide will be removed as found in the “Sequence” box.

When you push the blue button you get detailed information about a peptide. That means you are on the level of the single searches. Here you get more detailed information about the peptides. On that level the quantitative comparison is possible as well (the “Peak Area” column).



	Search	Score	Sequence	PeakArea	
☑	1	45.59	.TVM%E*NFVAFVD*K.*		
☑	1	63.65	.TVM%E@NFVAFVD@K.@		
☑	1	34.19	.VPQVSTPTLVE@VSR.@		
☑	1	49.59	.VPQVSTPTLVE*VSR.*		
☑	1	24.34	.YICD@NQD@TISSK.@		
☑	1	45.04	.YICD*NQD*TISSK.*		
☑	1	26.62	.YICDNQD@TISSK.@		
☑	1	34.54	.YLYE*IAR.*		
☑	1	26.44	.YLYE@IAR.@		

Peptidehits per page: [15] 25 50 100

69 Peptidehits found << Previous | Page 5 of 5 | go to page go

Details from YLYEIAR

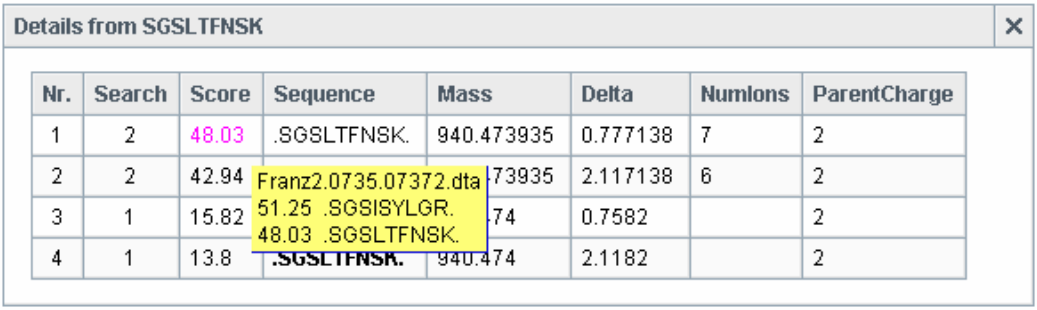
Nr.	Search	Score	Sequence	Mass	Delta	NumIons	ParentCharge	PeakArea
1	1	35.05	.YLYE*IAR.*	993.613782	0.537291	6	2	8.7043128E7
2	1	34.54	.YLYE*IAR.*	993.613782	0.197291	6	2	8.7043128E7
3	1	33.37	.YLYE*IAR.*	993.613782	-0.022709	6	2	8.7043128E7
4	1	28.85	.YLYE*IAR.*	993.613782	2.497291	5	2	8.7043128E7

Details from YLYEIAR

Nr.	Search	Score	Sequence	Mass	Delta	NumIons	ParentCharge	PeakArea
1	1	32.99	.YLYE@IAR.@	983.556501	0.304572	6	2	4.1418732E7
2	1	32.88	.YLYE@IAR.@	983.556501	0.564572	6	2	4.1418732E7
3	1	26.44	.YLYE@IAR.@	983.556501	0.674572	5	2	4.1418732E7

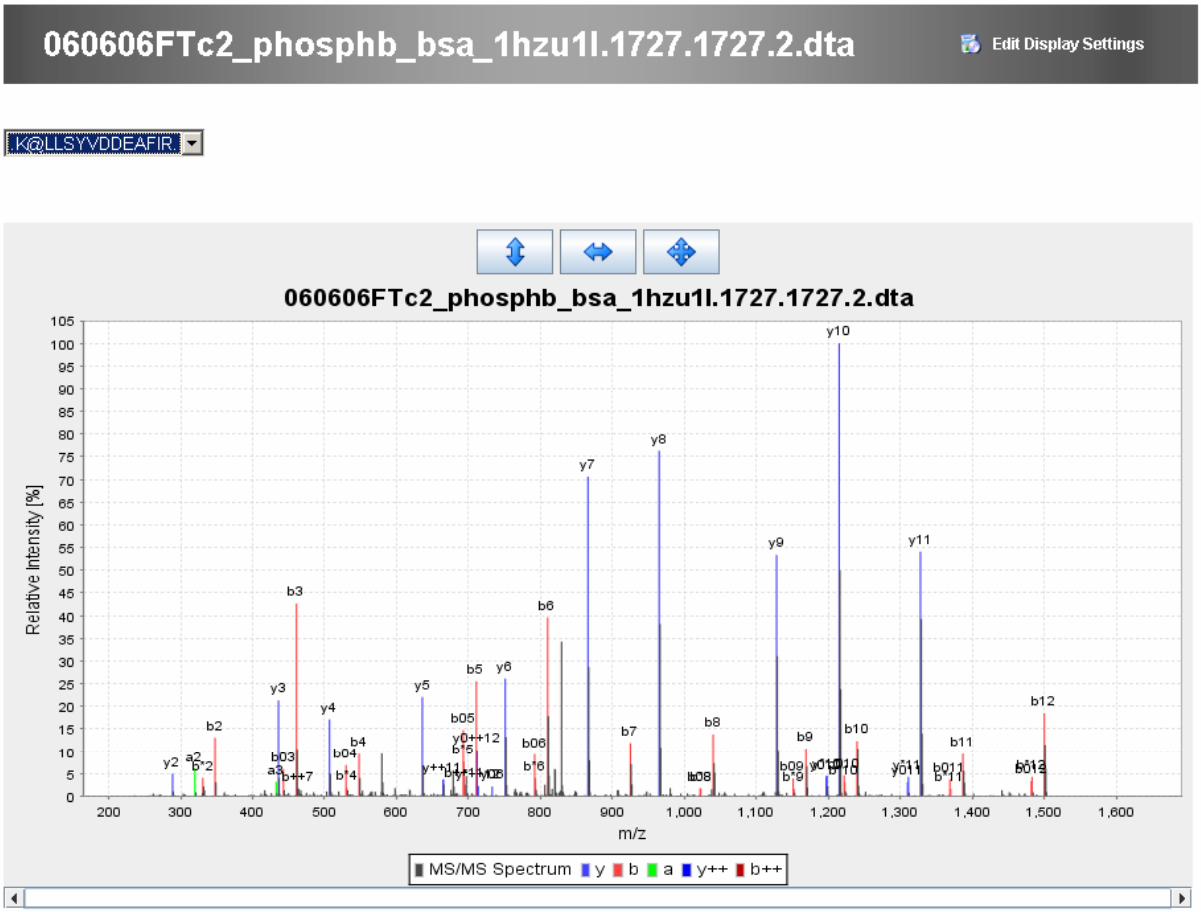
Return

When you move your mouse over one entry of the column “Search”, “Sequence” or “Score” a tooltip with the hits will be displayed.

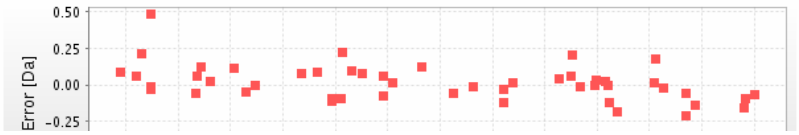


When you click on one of the entries with the tooltip a window pops up with the corresponding spectrum, so that manual validation is possible (see 7.4).

7.4 Spectrum View:

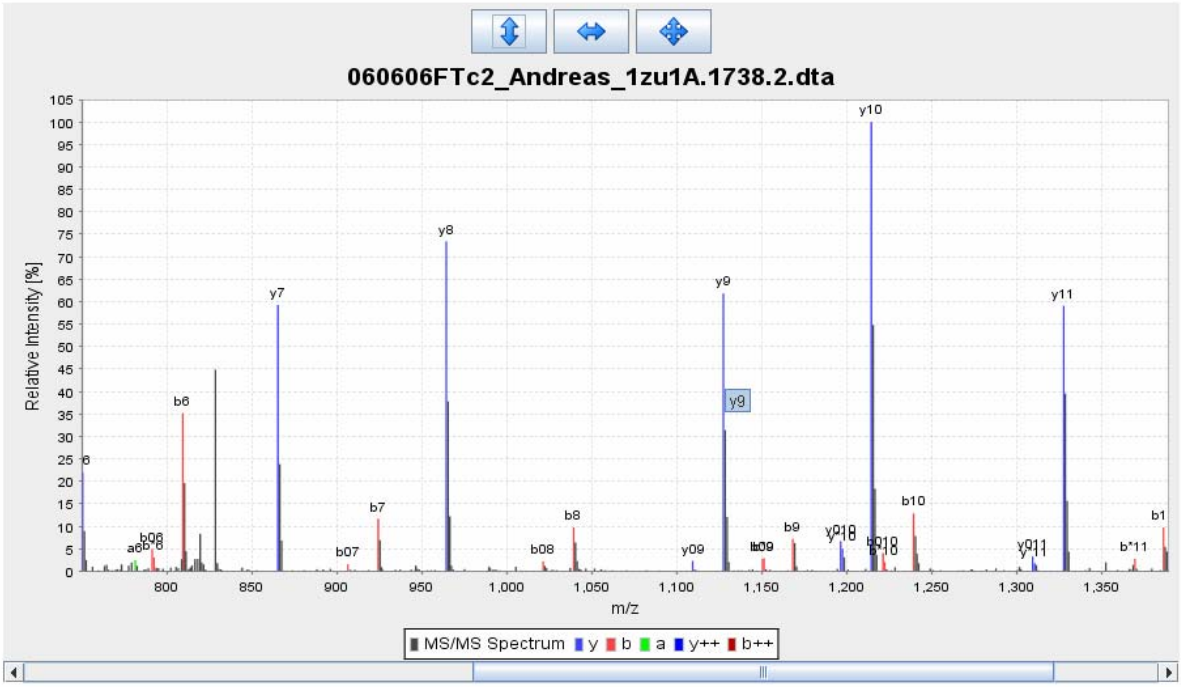


	a	b	b*	b0	b++	b*++	b0++		y	y*	y0	y++	y*++	y0++	
1	206.12	234.12	217.09	216.11	117.56	109.05	108.56	K							13
2	319.21	347.2	330.18	329.19	174.1	165.59	165.1	L	1440.73	1423.71	1422.72	720.87	712.35	711.86	12
3	432.29	460.29	443.26	442.28	230.64	222.13	221.64	L	1327.65	1310.62	1309.64	664.33	655.81	655.32	11
4	519.32	547.32	530.29	529.31	274.16	265.65	265.16	S	1214.56	1197.54	1196.55	607.78	599.27	598.78	10
5	682.39	710.38	693.35	692.37	355.69	347.18	346.69	Y	1127.53	1110.51	1109.52	564.27	555.75	555.26	9
6	781.45	809.45	792.42	791.44	405.23	396.71	396.22	V	964.47	947.44	946.46	482.74	474.22	473.73	8
7	896.48	924.48	907.45	906.47	462.74	454.23	453.73	D	865.4	848.37	847.39	433.2	424.69	424.2	7
8	1011.51	1039.5	1022.48	1021.49	520.25	511.74	511.25	D	750.37	733.35	732.36	375.69	367.17	366.68	6
9	1140.55	1168.55	1151.52	1150.54	584.77	576.26	575.77	E	635.35	618.32	617.34	318.17	309.66	309.17	5
10	1211.59	1239.58	1222.56	1221.57	620.29	611.78	611.29	A	506.3	489.28	488.29	253.65	245.14	244.65	4
11	1358.66	1386.65	1369.63	1368.64	693.83	685.31	684.82	F	435.27	418.24	417.26	218.13	209.62	209.13	3
12	1471.74	1499.74	1482.71	1481.73	750.37	741.86	741.36	I	288.2	271.17	270.19	144.6	136.09	135.6	2
13								R	175.11	158.09	157.1	88.06	79.55	79.05	1



With “Edit Display Settings” you can select the series you want to be displayed. You can save your own display settings like in all the other pages.
With the select box below the “Edit Display Settings” box you can switch between the found hits.
Then there is a Java Applet with the spectrum (see 7.4.1) and after the spectrum view a box with calculated masses of the fragments is added. At the bottom of the page the mass error of the single hits of the different series is displayed.

7.4.1 The spectrum viewer:



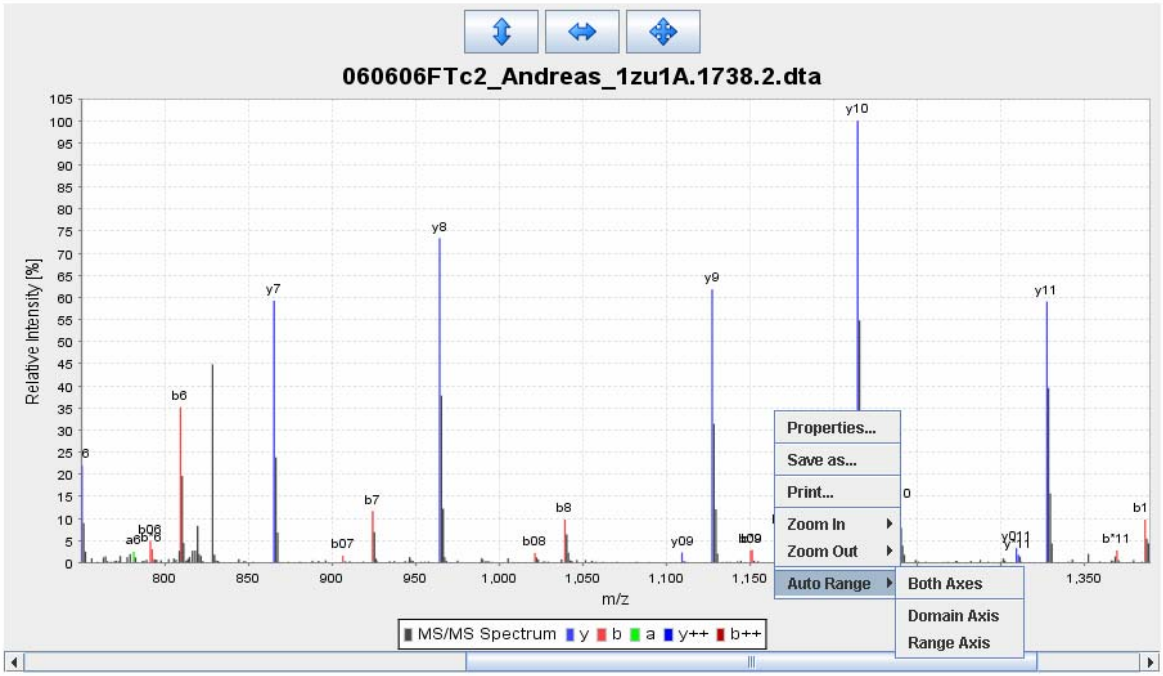
The not assigned peaks are displayed in red. The assigned fragment name is written on the top of the peak. If you hover your mouse over one peak the name will be displayed in a tooltip as well. You can zoom into your spectrum and scroll the x-axis with the bar at the bottom.

 : zooms out the y-axis

 : zooms out the x-axis

 : zooms out both axes

When you first click on the spectrum and then click with the right mouse button you will get a popup window where you have additional features:



You can print your actual zoom scan. In the “Properties…” you can customize your font and other settings.