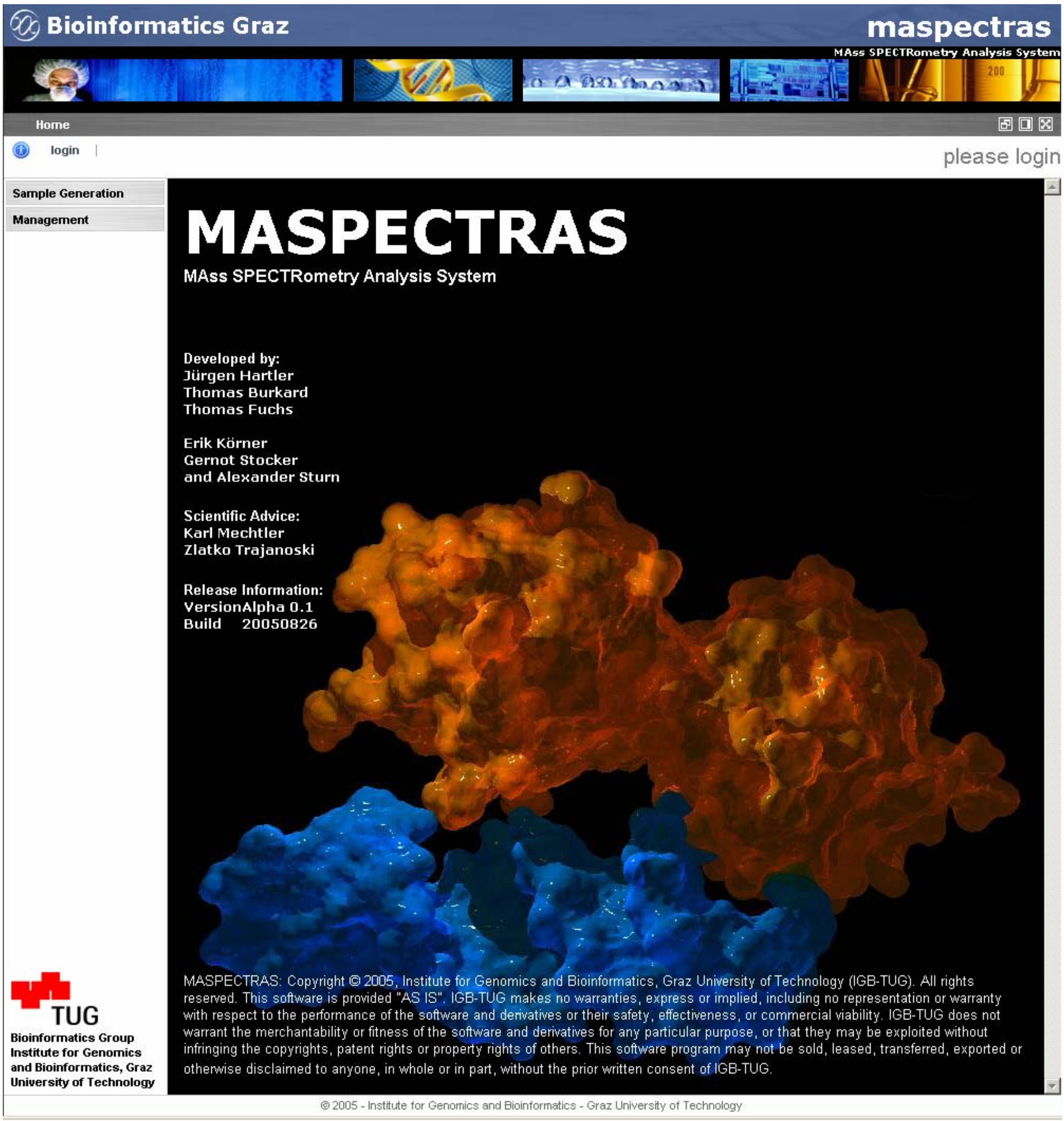
MASPECTRAS

Users Guide

1. General Information:



MASPECTRAS

MAss SPECTRometry Analysis System

Developed by:
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Zlatko Trajanoski

Release Information:
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Build 20050826

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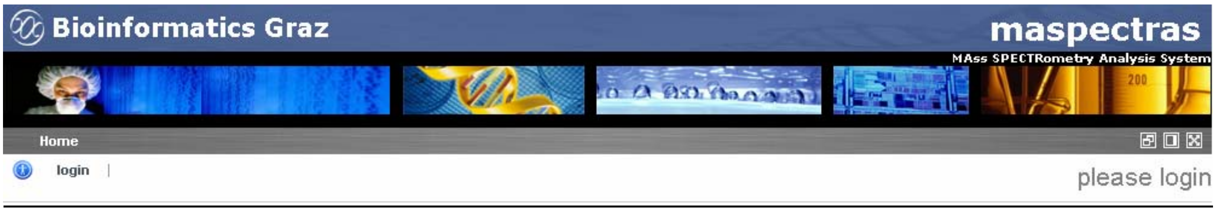
This will be your first impression of MASPECTRAS.
The main view is divided into 3 sections:

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:

please login

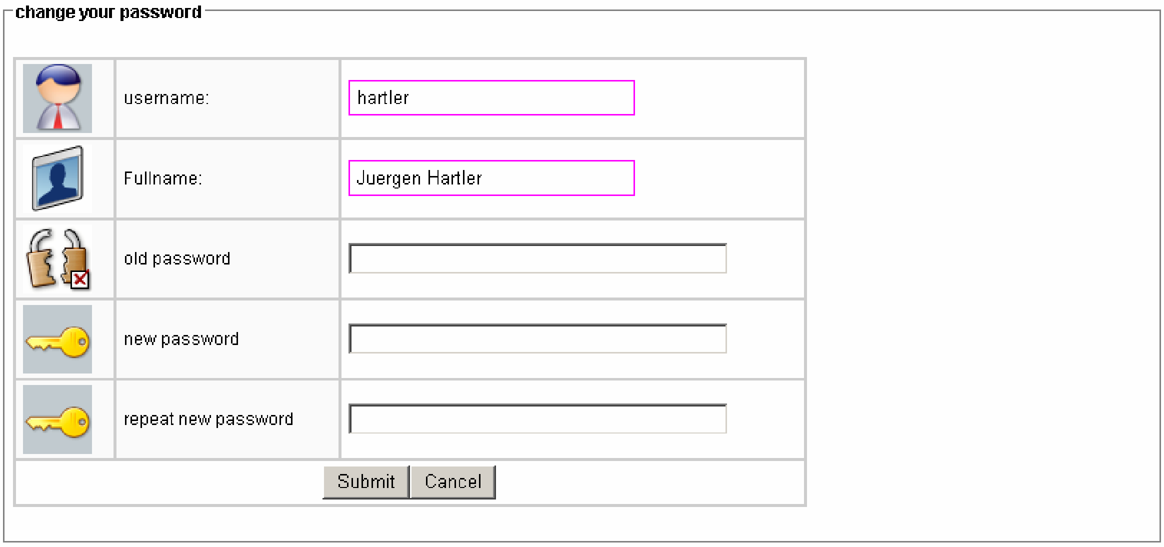
gives the possibility to log in

If you are logged in:

You are logged in as Juergen Hartler

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:



username: hartler

Fullname: Juergen Hartler

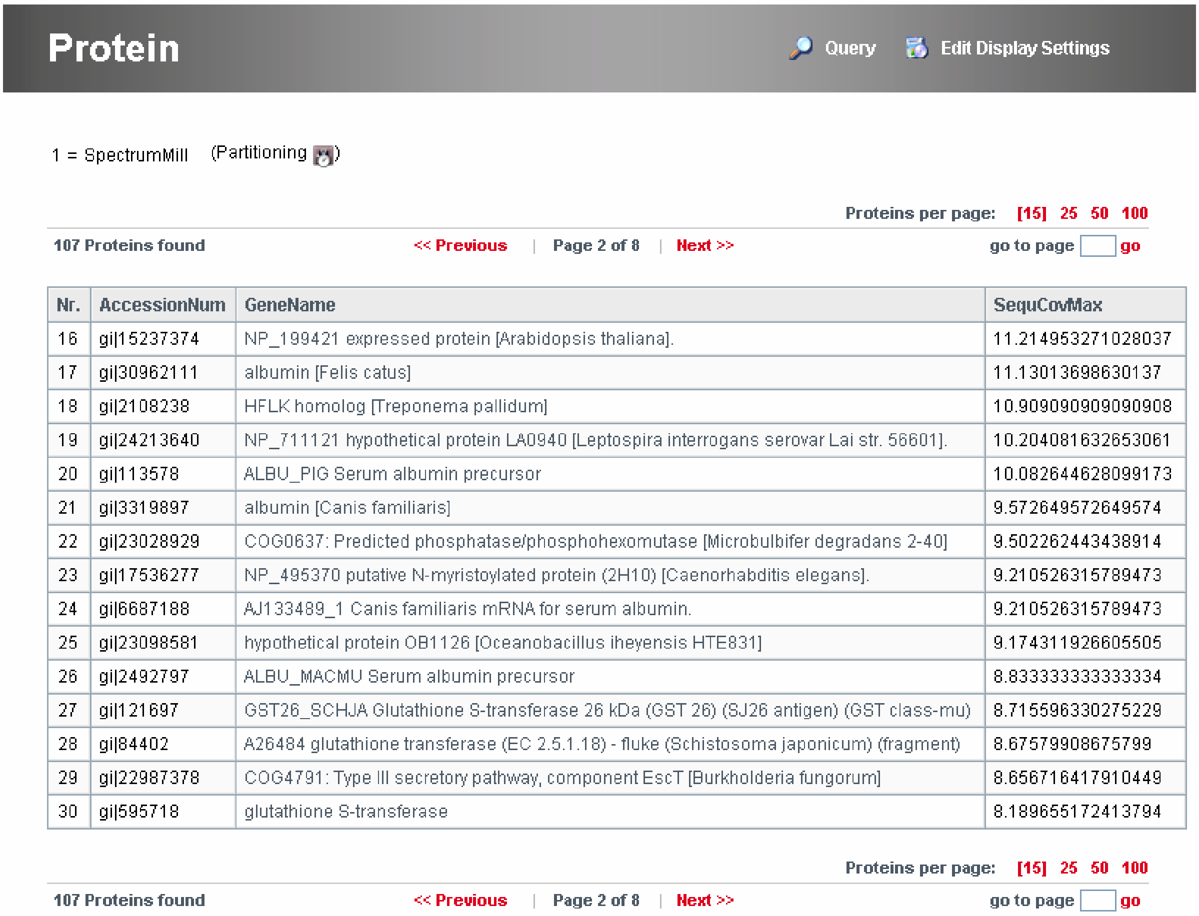
old password

new password

repeat new 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:



1 = SpectrumMill (Partitioning)

107 Proteins found

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

107 Proteins found

The general presentation of the data in MASPECTRAS looks like in the figure above.

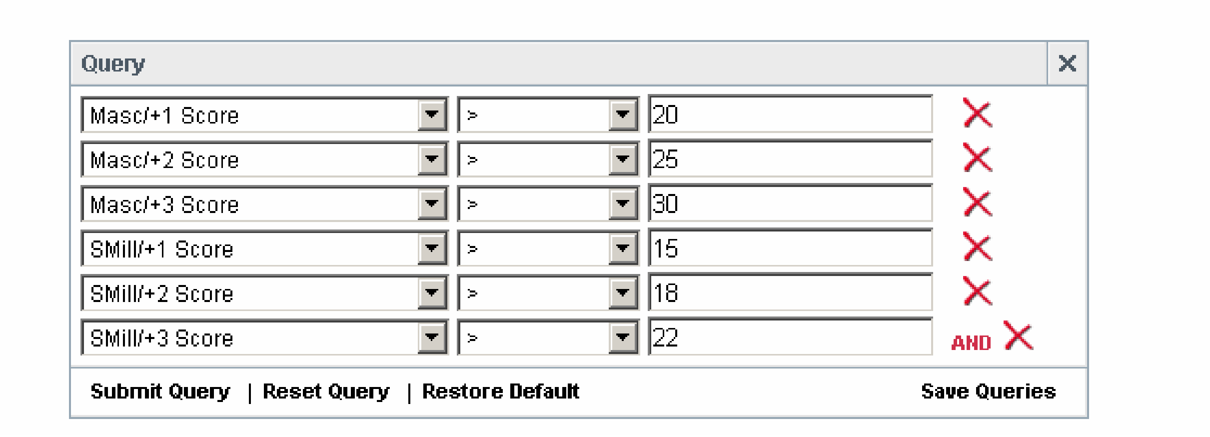
In the header section there are 2 links:

- 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:



Masc/+1 Score > 20
Masc/+2 Score > 25
Masc/+3 Score > 30
SMill/+1 Score > 15
SMill/+2 Score > 18
SMill/+3 Score > 22

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

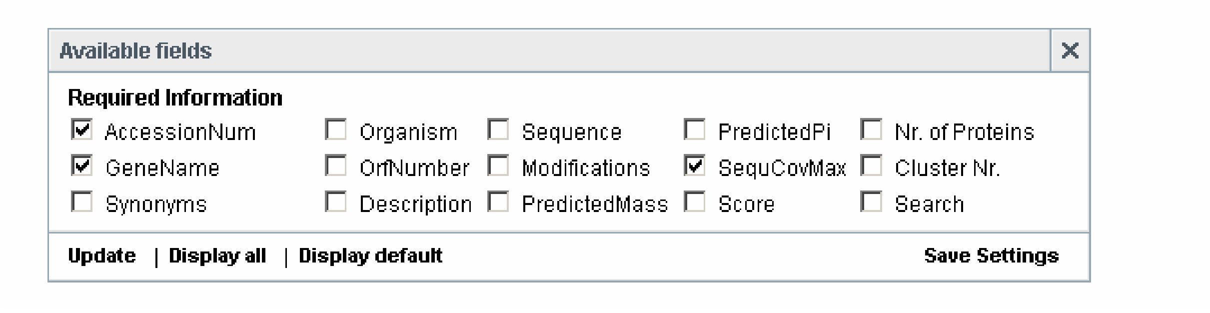
The button "Submit Query" submits the entered query and changes the view on the data correspondingly.

"Reset Query" removes all entered queries and submits a query without any user-defined restrictions.

Restore Default" submits a set of queries which have been saved.

"Save Queries" saves the actually entered set of queries to the database and submits them. If one set of queries is saved your data on that page will always be filtered with this set by default (unless you change the queries).

1.2.2 Customizable display:

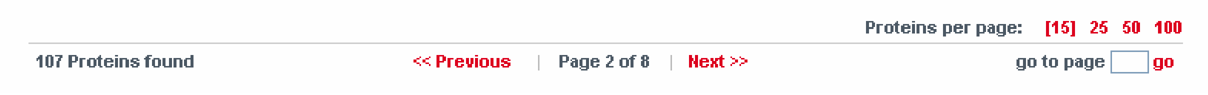


Required Information

☑ AccessionNum
☑ GeneName
☐ Synonyms
☐ Organism
☐ OrfNumber
☐ Description
☐ Sequence
☐ Modifications
☐ PredictedMass
☐ PredictedPi
☑ SequCovMax
☐ Score
☐ Nr. of Proteins
☐ Cluster Nr.
☐ Search

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.

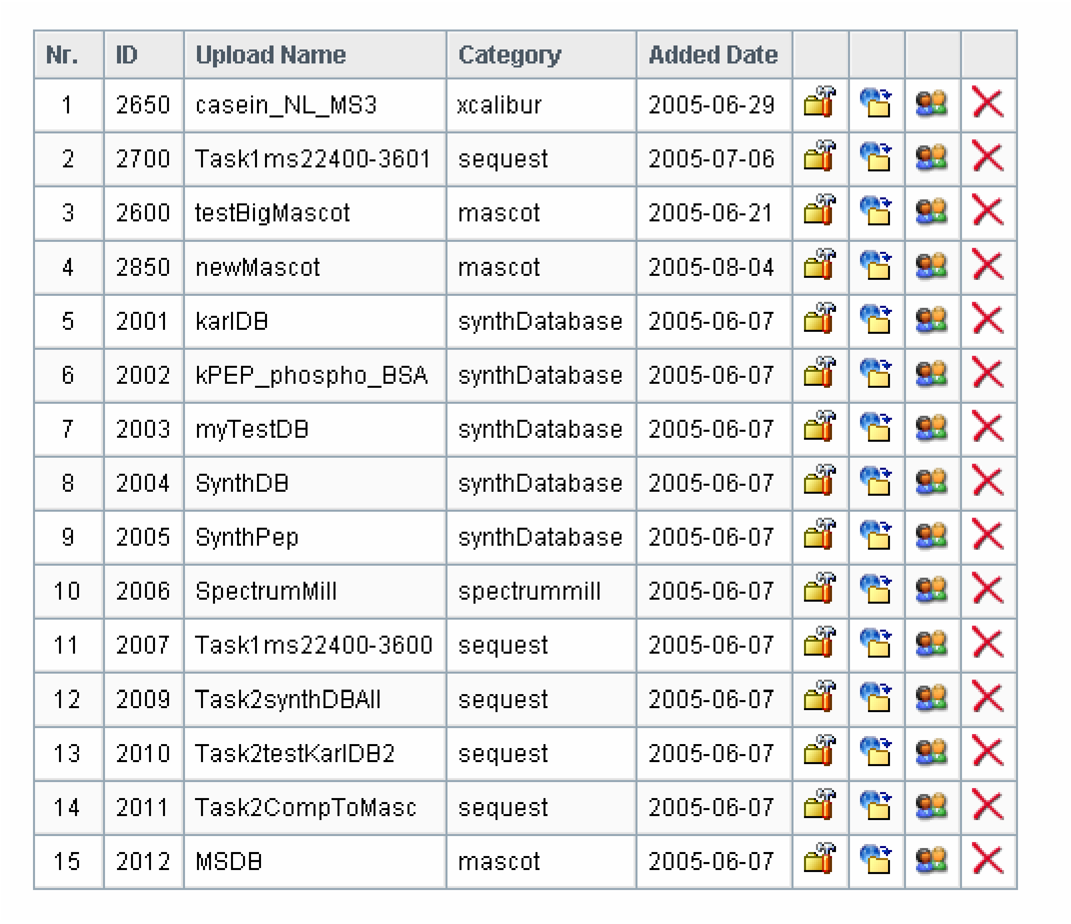
1.2.3 Scrolling bar:



Proteins per page: [15] 25 50 100

107 Proteins found | << Previous | Page 2 of 8 | Next >> | go to page go

On the left the scrolling bar indicates 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. You can also jump to any page you like. (At the right side you can define the size of your page by your own and you can enter the page number and push the “go” button to jump to your desired page.)



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 out of the following parts:

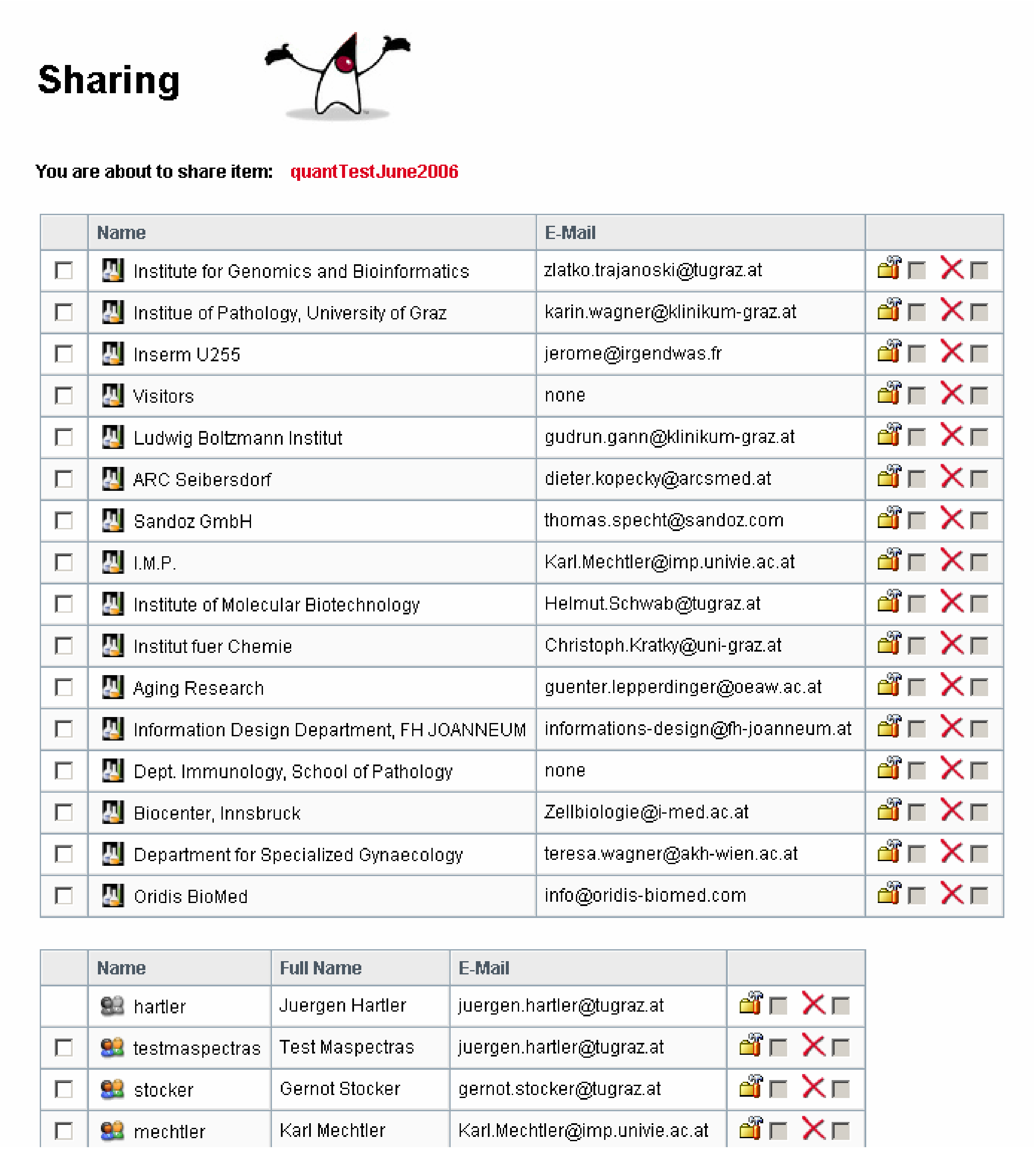
- The header: if you hover your mouse above the column-name and the colour changes to blue, you can sort by this column
- The number in the first column indicates the hit number of the entry corresponding to the order you sorted your data
- Links to data connected to the entries are normally located 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 to them:



Sharing

You are about to share item: quantTestJune2006

	Name	E-Mail	
☐	Institute for Genomics and Bioinformatics	zlatko.trajanoski@tugraz.at	🖉 ☐ ✕ ☐
☐	Institue of Pathology, University of Graz	karin.wagner@klinikum-graz.at	🖉 ☐ ✕ ☐
☐	Inserm U255	jerome@irgendwas.fr	🖉 ☐ ✕ ☐
☐	Visitors	none	🖉 ☐ ✕ ☐
☐	Ludwig Boltzmann Institut	gudrun.gann@klinikum-graz.at	🖉 ☐ ✕ ☐
☐	ARC Seibersdorf	dieter.kopecky@arcsmed.at	🖉 ☐ ✕ ☐
☐	Sandoz GmbH	thomas.specht@sandoz.com	🖉 ☐ ✕ ☐
☐	I.M.P.	Karl.Mechtler@imp.univie.ac.at	🖉 ☐ ✕ ☐
☐	Institute of Molecular Biotechnology	Helmut.Schwab@tugraz.at	🖉 ☐ ✕ ☐
☐	Institut fuer Chemie	Christoph.Kratky@uni-graz.at	🖉 ☐ ✕ ☐
☐	Aging Research	guenter.lepperdinger@oeaw.ac.at	🖉 ☐ ✕ ☐
☐	Information Design Department, FH JOANNEUM	informations-design@fh-joanneum.at	🖉 ☐ ✕ ☐
☐	Dept. Immunology, School of Pathology	none	🖉 ☐ ✕ ☐
☐	Biocenter, Innsbruck	Zellbiologie@i-med.ac.at	🖉 ☐ ✕ ☐
☐	Department for Specialized Gynaecology	teresa.wagner@akh-wien.ac.at	🖉 ☐ ✕ ☐
☐	Oridis BioMed	info@oridis-biomed.com	🖉 ☐ ✕ ☐

	Name	Full Name	E-Mail	
	hartler	Juergen Hartler	juergen.hartler@tugraz.at	🖉 ☐ ✕ ☐
☐	testmaspectras	Test Maspectras	juergen.hartler@tugraz.at	🖉 ☐ ✕ ☐
☐	stocker	Gernot Stocker	gernot.stocker@tugraz.at	🖉 ☐ ✕ ☐
☐	mechtler	Karl Mechtler	Karl.Mechtler@imp.univie.ac.at	🖉 ☐ ✕ ☐

When you select a user or an institute the checkboxes at 🖉 and ✕ are enabled here 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 this one:

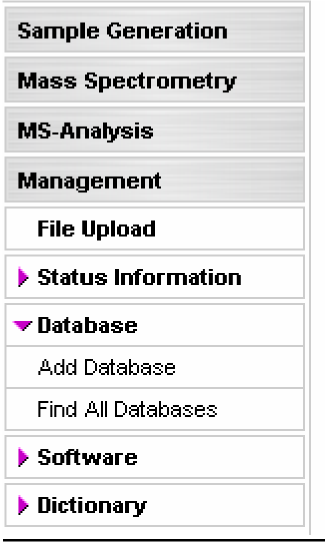
Ionsource: myElectrosprayIonsource

When 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”.

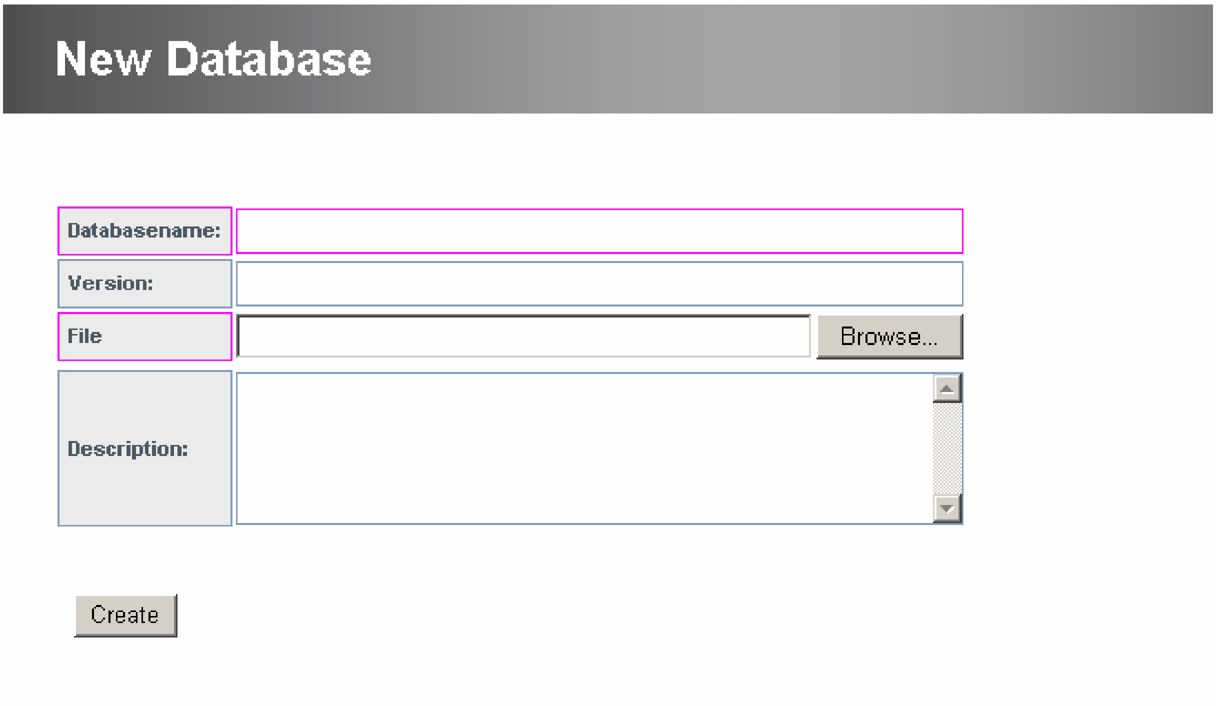
2. Management Section:

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.

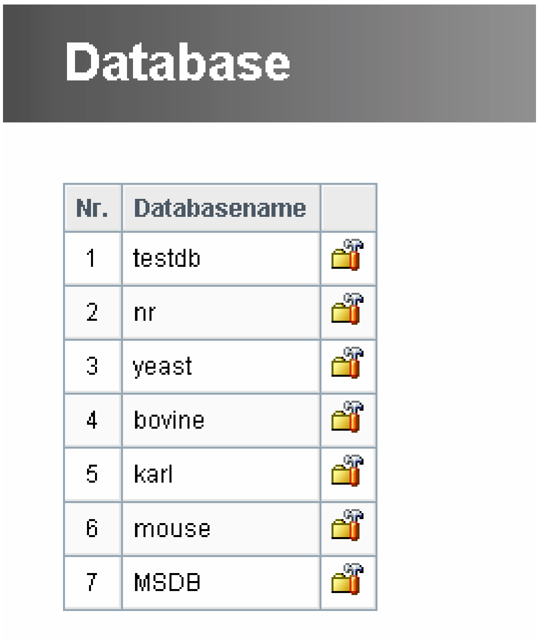


With the “Add Database” you can add a new database.



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.

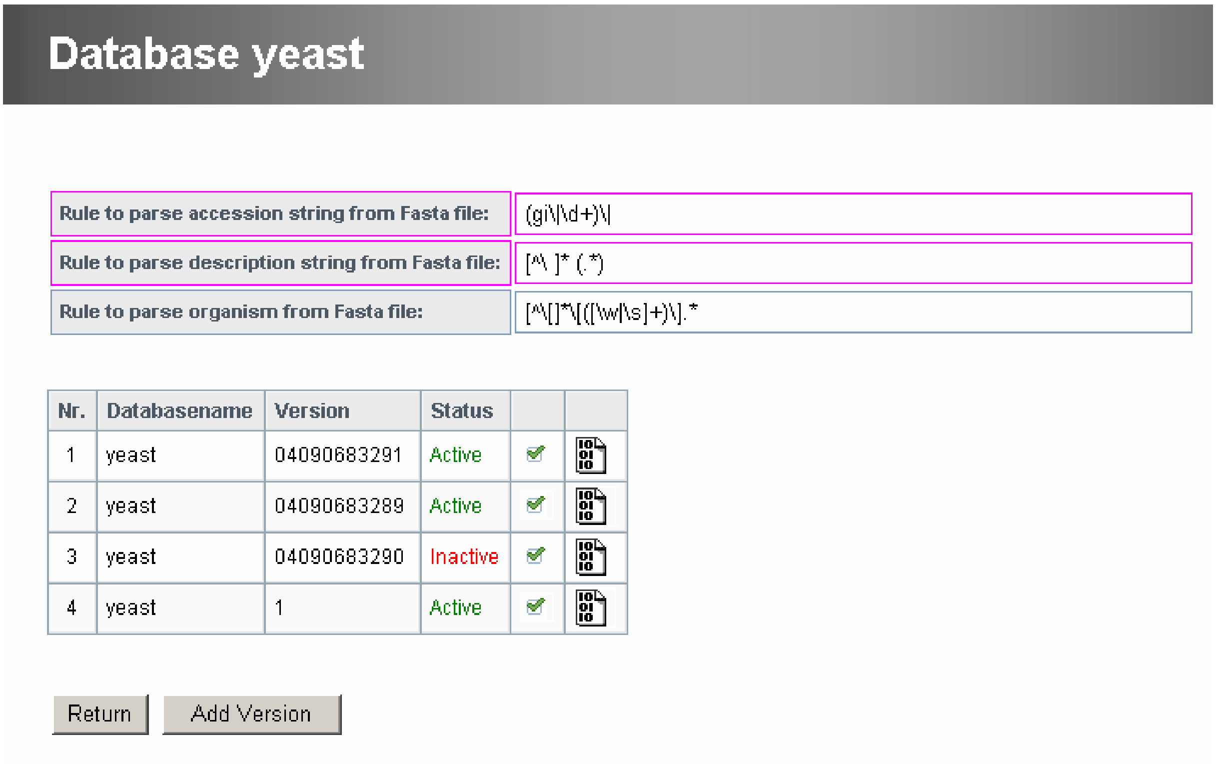
With the “Find All Databases” you get an overview of all your databases.



Database

Nr.	Databasename	
1	testdb	
2	nr	
3	yeast	
4	bovine	
5	karl	
6	mouse	
7	MSDB	

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



Database yeast

Rule to parse accession string from Fasta file: `(gi\|\d+)\|`

Rule to parse description string from Fasta file: `[^\ ]* (.*)`

Rule to parse organism from Fasta file: `[^\[]*\[([\w|\s]+)\].*`

Nr.	Databasename	Version	Status		
1	yeast	04090683291	Active	✓	
2	yeast	04090683289	Active	✓	
3	yeast	04090683290	Inactive	✓	
4	yeast	1	Active	✓	

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.

The database can have the following stati:

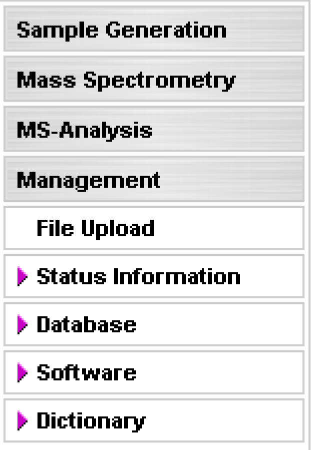
Active : The database is active and can be used for file parsing.

Indexing : This database is indexing. (This page is not refreshed automatically at the moment, you have to go by hand to this page to see if it is already active)

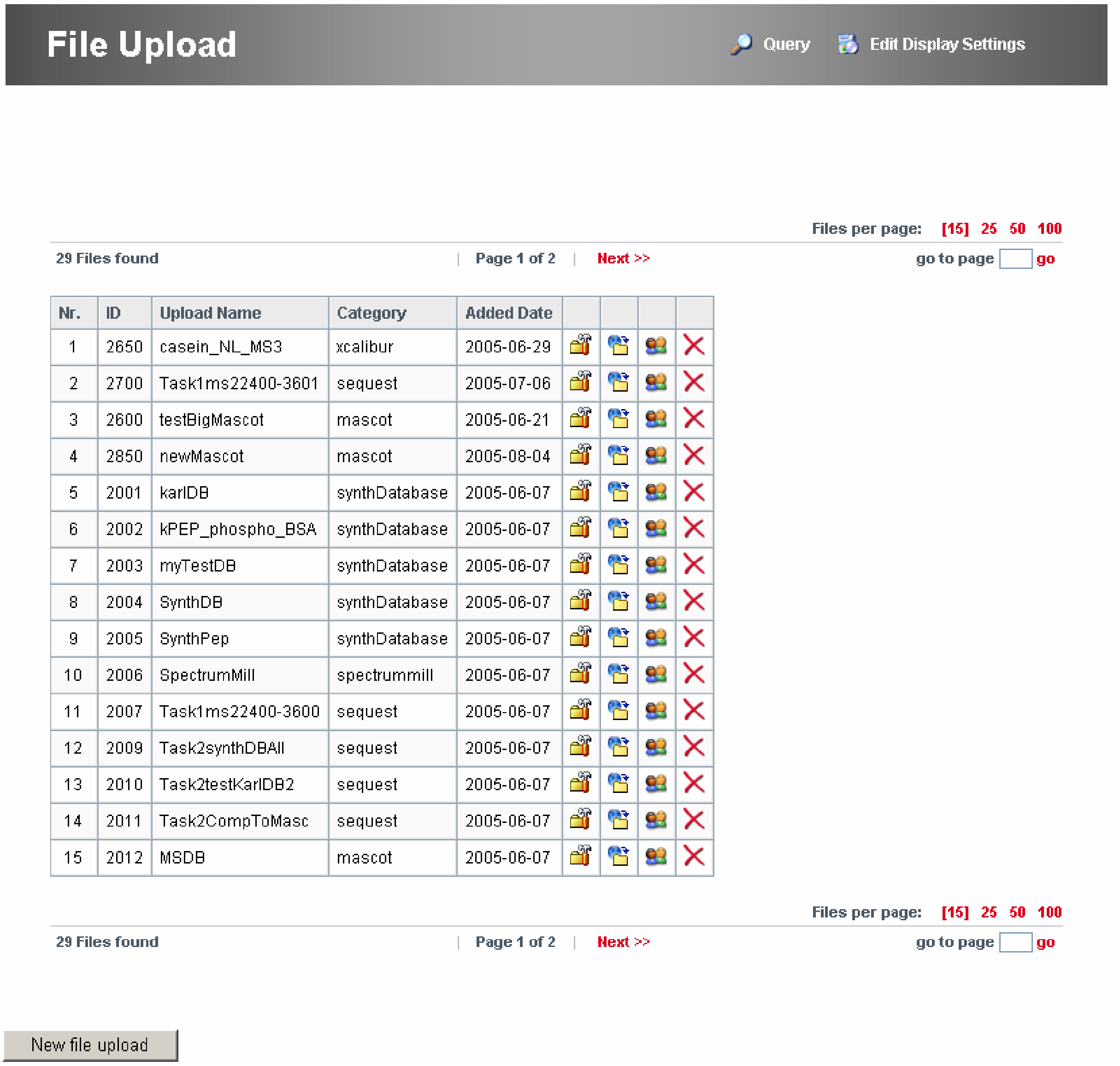
Inactive : The database has not been indexed or something at the indexing has gone wrong

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 change in a running instance, you have to be aware that there are maybe 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:



Files per page: [15] 25 50 100

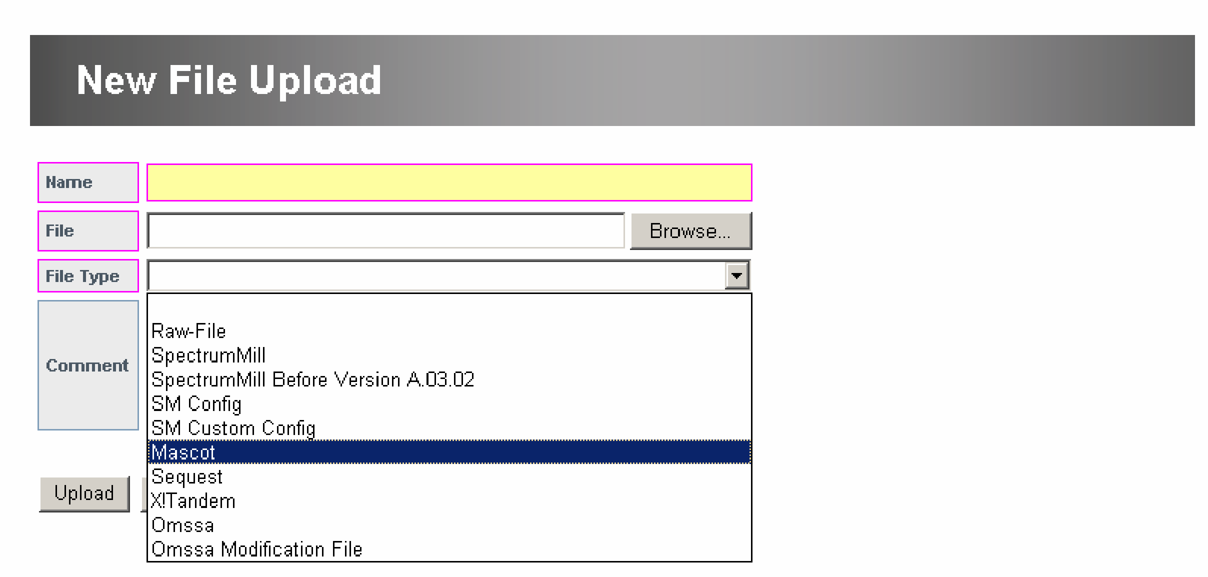
29 Files found | Page 1 of 2 | Next >> go to page go

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				✕

Files per page: [15] 25 50 100

29 Files found | Page 1 of 2 | Next >> go to page go

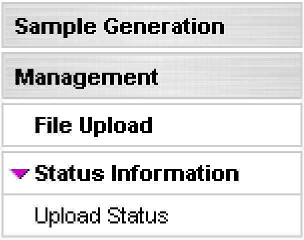
With “New file upload” you come to the upload page:



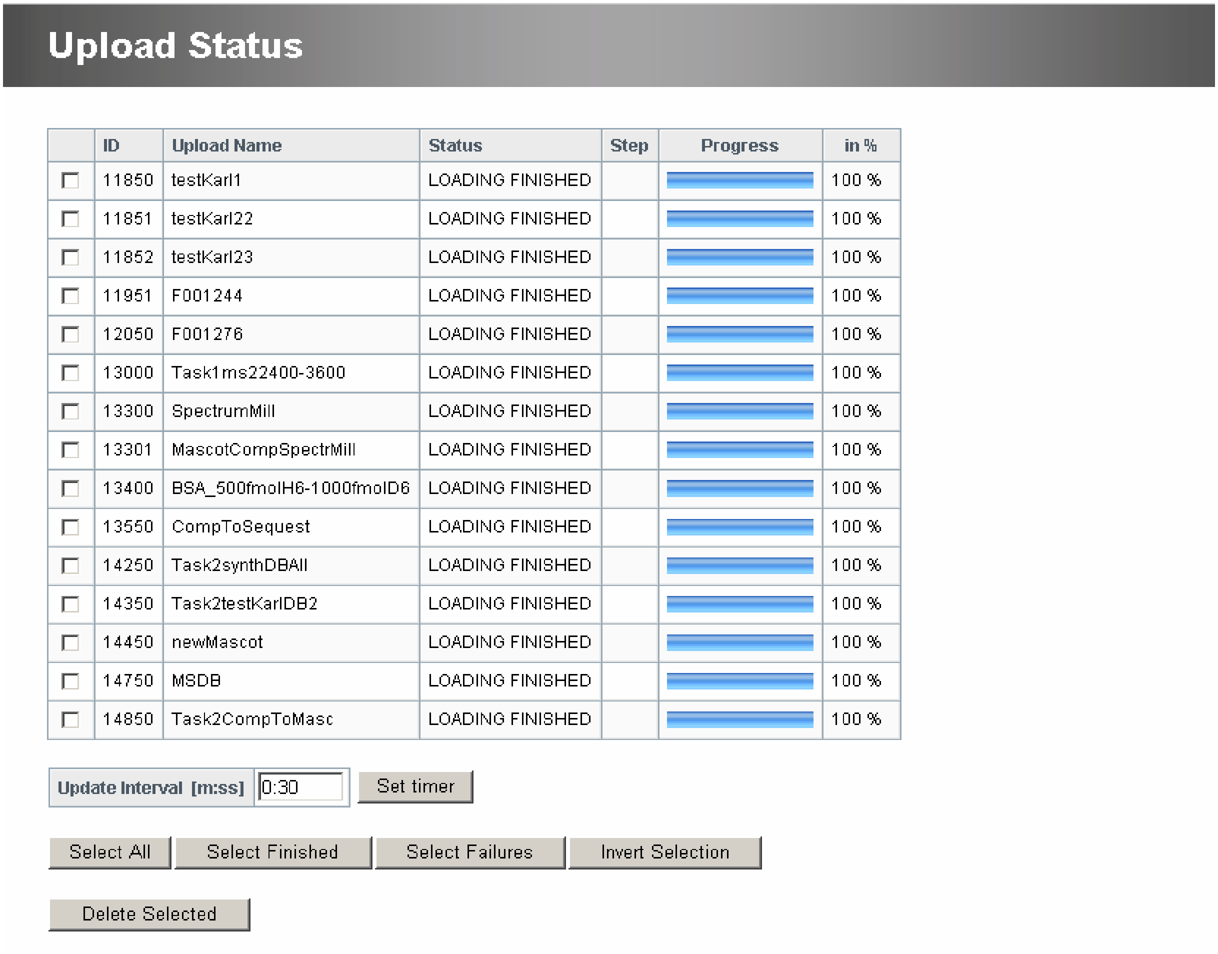
The important thing is that you have to add your file to the corresponding category. The Sequest-Files and SpectrumMill-Files must be uploaded in a *.zip directory. Spectrum Mill is differentiated in “Spectrum Mill” (new version) and “Spectrum Mill Before Version A.03.02” (old version). For the new version a SM Config File (your smconfig.xml file) is necessary. The SM Custom Config (your smconfig.custom.xml) is not mandatory, only 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 is 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.

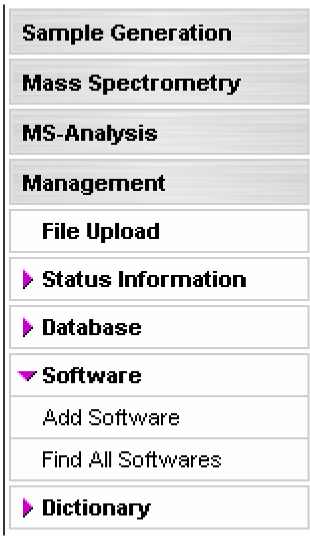


	ID	Upload Name	Status	Step	Progress	in %
☐	11850	testKarl1	LOADING FINISHED			100 %
☐	11851	testKarl22	LOADING FINISHED			100 %
☐	11852	testKarl23	LOADING FINISHED			100 %
☐	11951	F001244	LOADING FINISHED			100 %
☐	12050	F001276	LOADING FINISHED			100 %
☐	13000	Task1ms22400-3600	LOADING FINISHED			100 %
☐	13300	SpectrumMill	LOADING FINISHED			100 %
☐	13301	MascotCompSpectrMill	LOADING FINISHED			100 %
☐	13400	BSA_500fmolH6-1000fmolD6	LOADING FINISHED			100 %
☐	13550	CompToSequest	LOADING FINISHED			100 %
☐	14250	Task2synthDBAll	LOADING FINISHED			100 %
☐	14350	Task2testKarlDB2	LOADING FINISHED			100 %
☐	14450	newMascot	LOADING FINISHED			100 %
☐	14750	MSDB	LOADING FINISHED			100 %
☐	14850	Task2CompToMasc	LOADING FINISHED			100 %

Update Interval [m:ss] 0:30

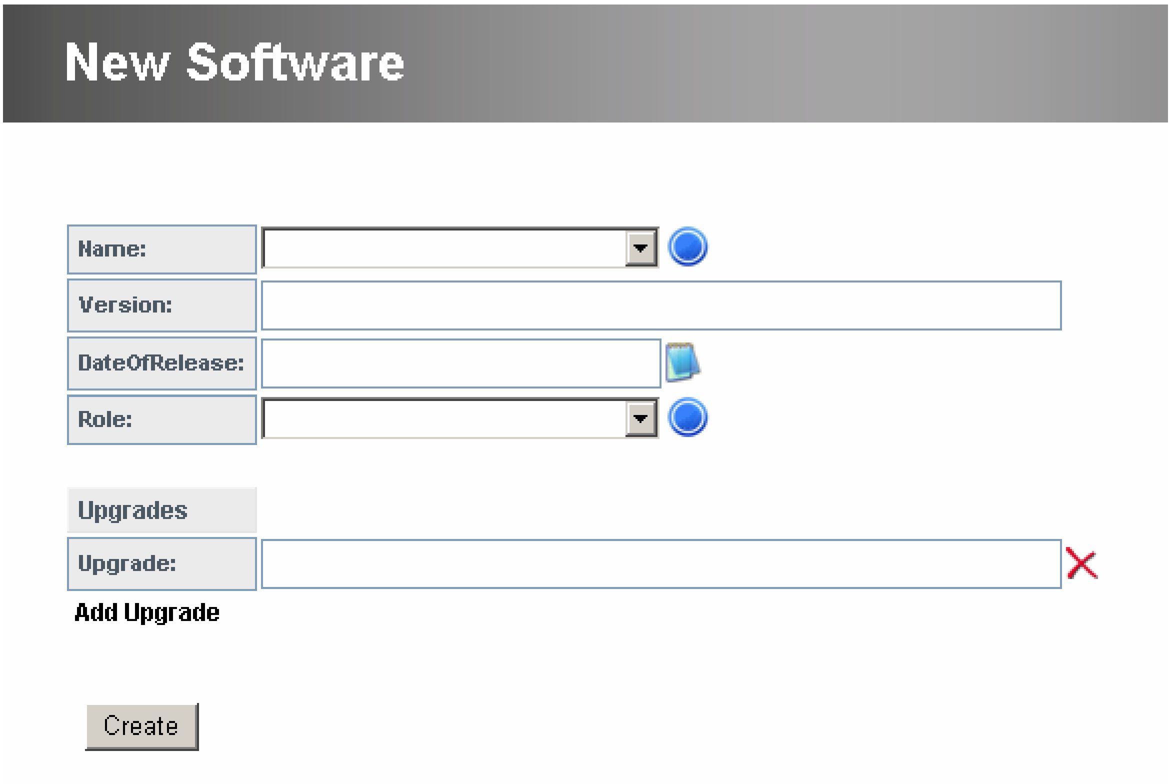
2.4 Software:

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 this point directly (e.g. see chapter 5.5 “Controlsoftware”).

With the “Add Software” you can add a new software.



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

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

1 Softwares found | Page 1 of 1 |

Nr.	Name	Version	Role			
1	XCalibur	2.0	massSpectrometrySoftware			✗

1 Softwares found | Page 1 of 1 |

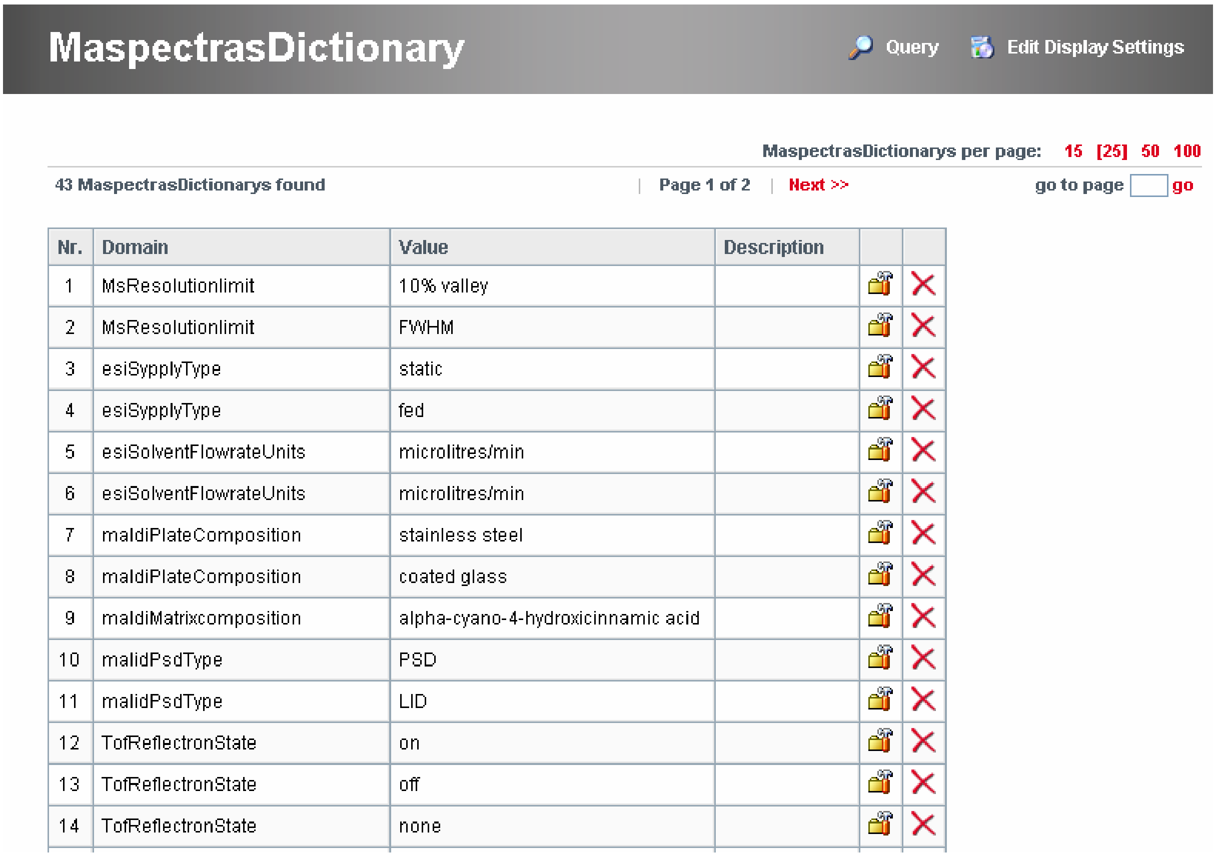
2.5 Dictionary:

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.



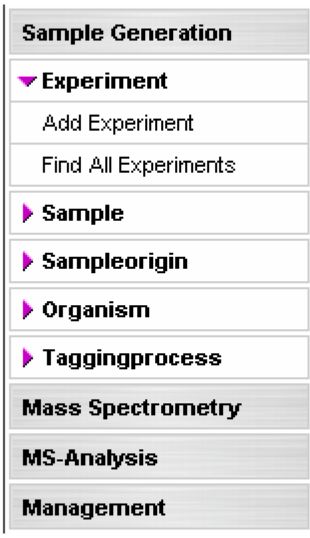
43 MaspectrasDictionarys found

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			

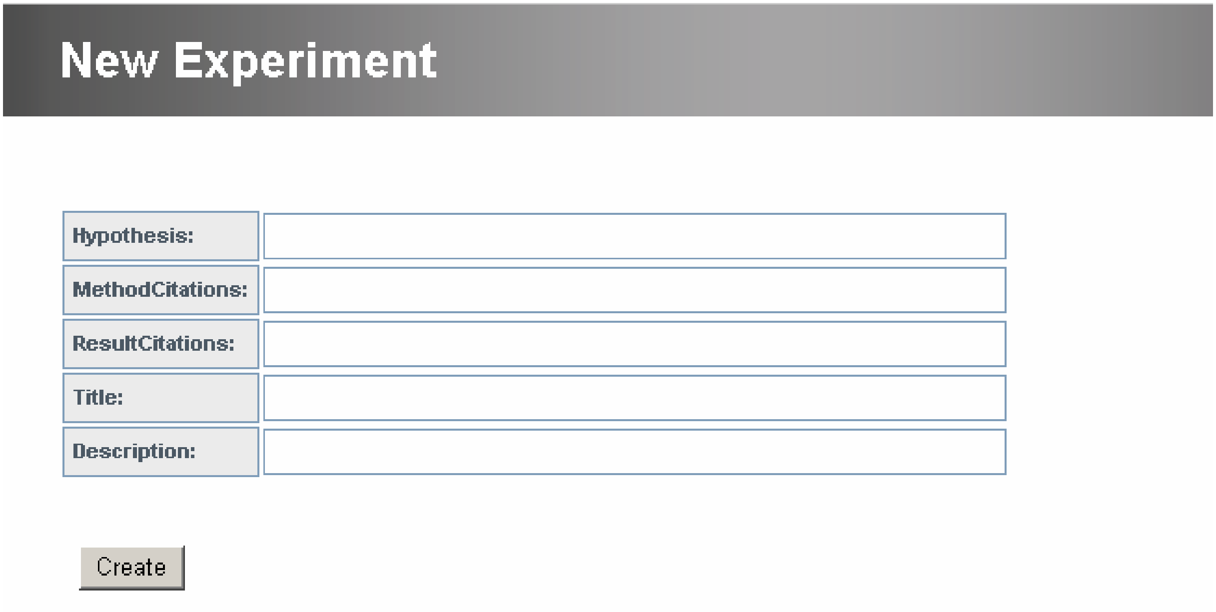
3. Sample Description:

3.1 Experiment:

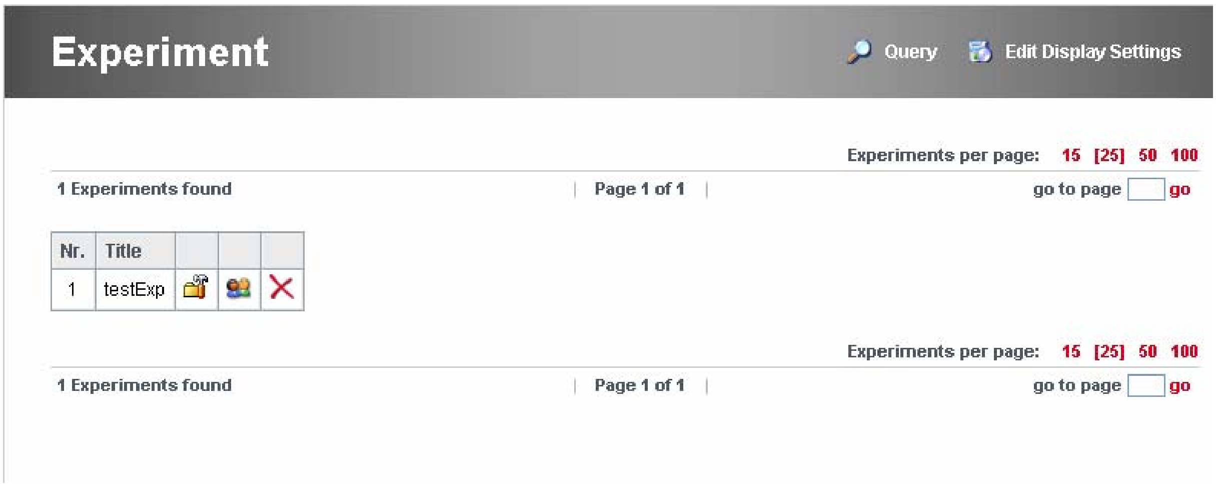
By clicking Sample Generation->Experiment you reach the experiment section.



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



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



1 Experiments found | Page 1 of 1 |

Nr.	Title			
1	testExp			✕

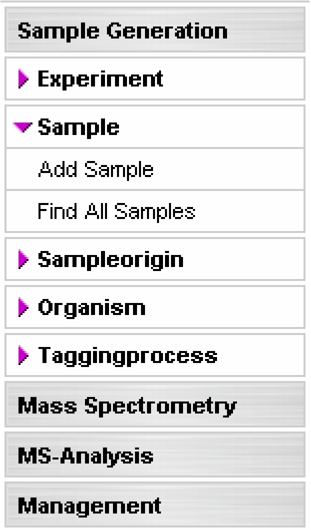
1 Experiments found | Page 1 of 1 |

3.2 Sample:

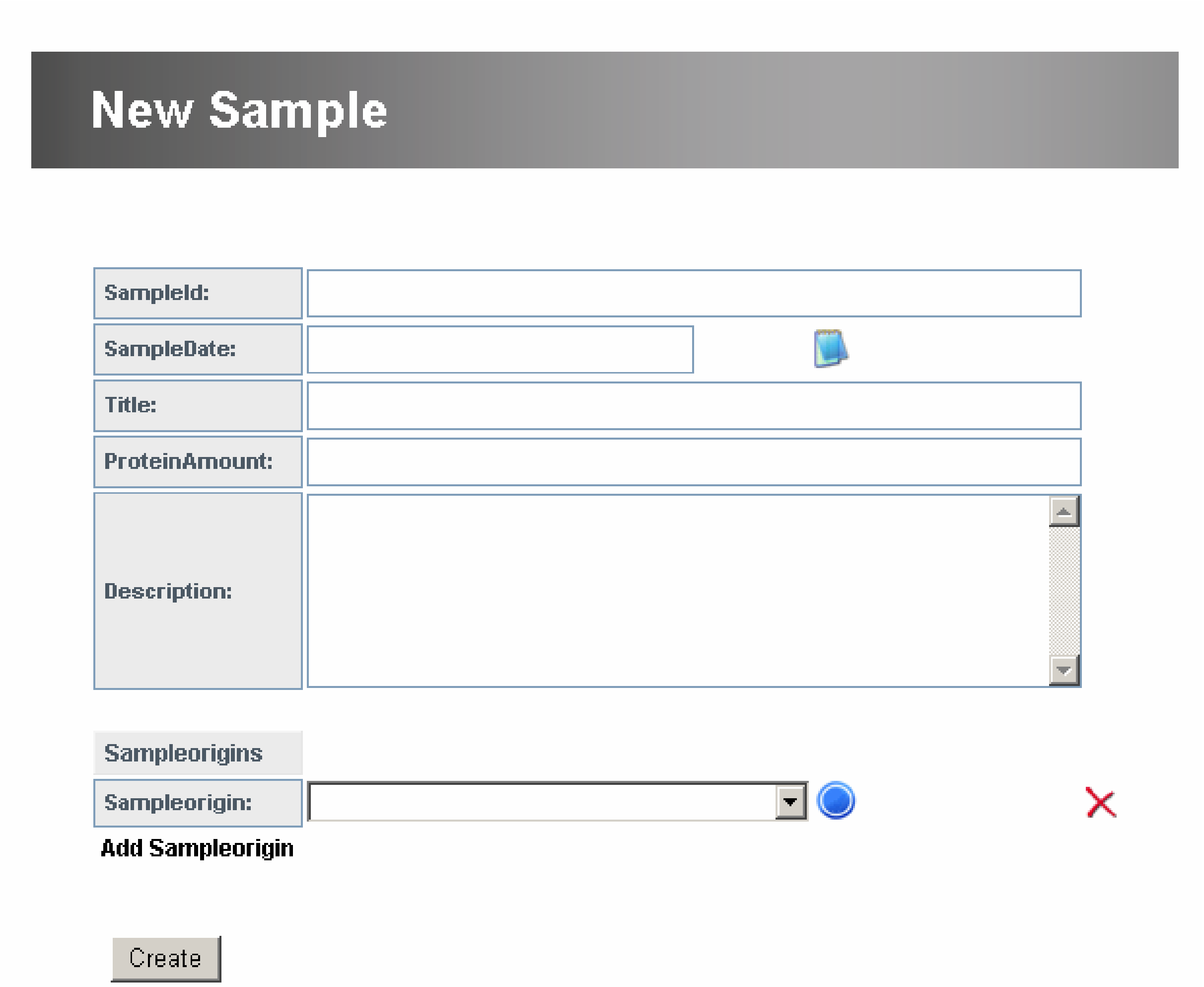
There are 2 ways to generate your sample:

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.

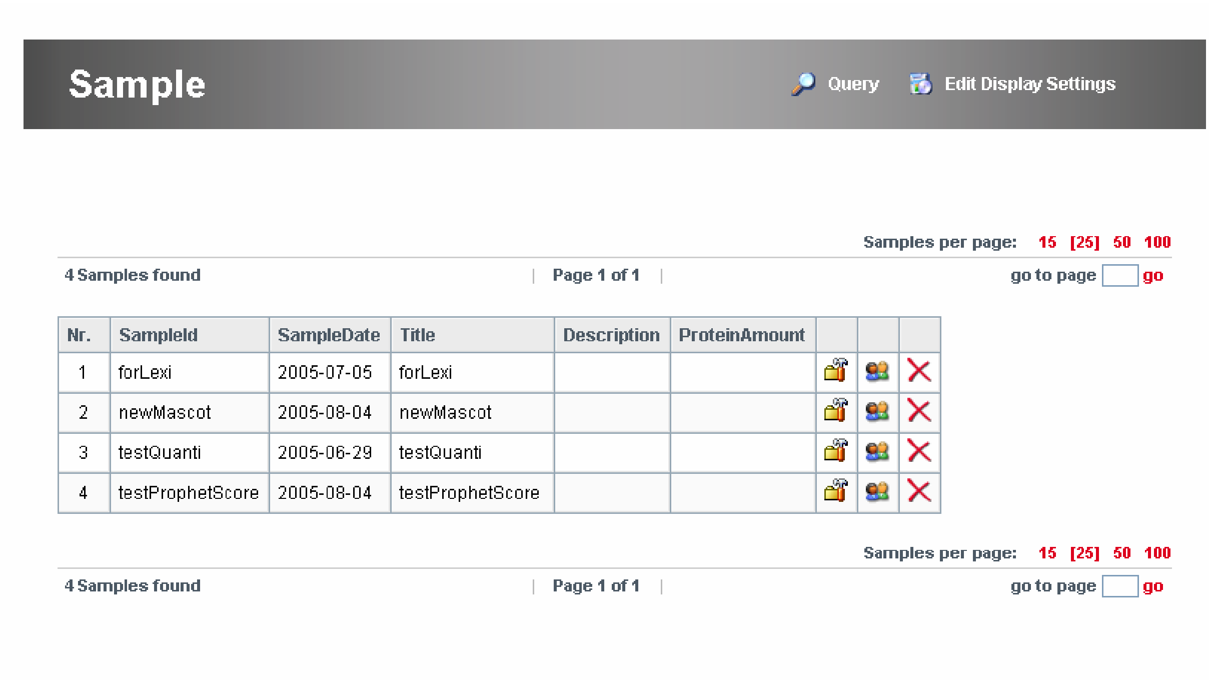


With the “Add Sample” you can add a new sample:



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:



4 Samples found | Page 1 of 1 |

Nr.	SampleId	SampleDate	Title	Description	ProteinAmount			
1	forLexi	2005-07-05	forLexi					
2	newMascot	2005-08-04	newMascot					
3	testQuanti	2005-06-29	testQuanti					
4	testProphetScore	2005-08-04	testProphetScore					

4 Samples found | Page 1 of 1 |

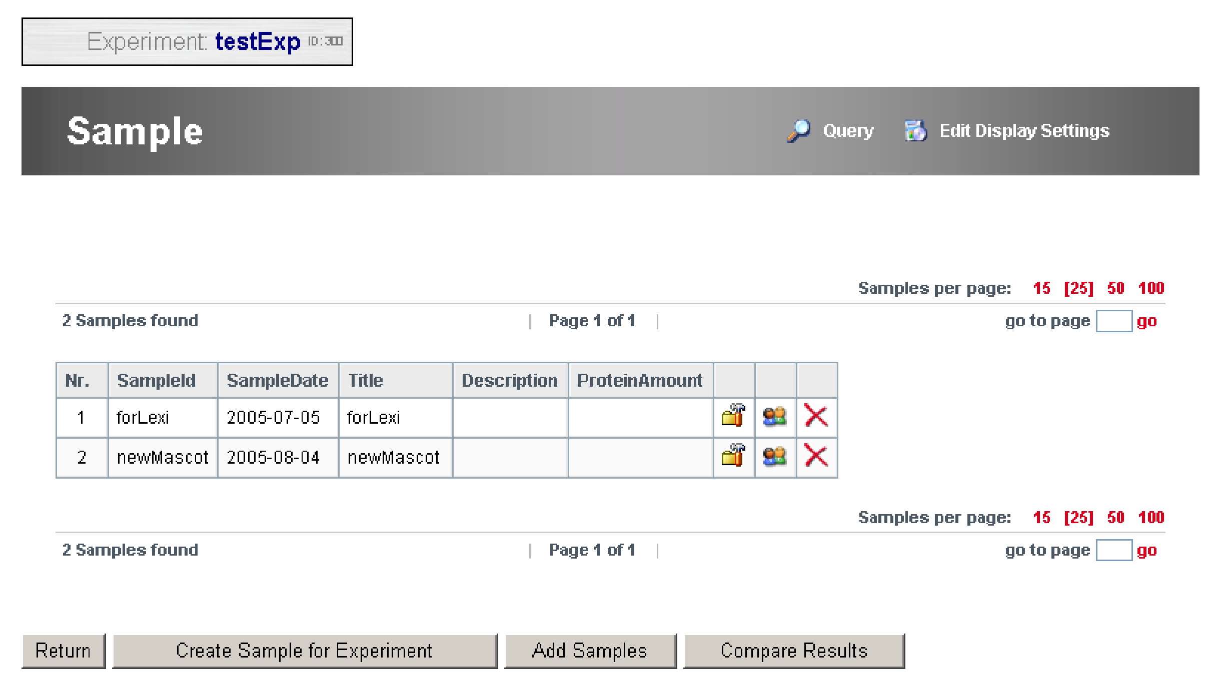
3.2.2 Sample over experiment:

1 Experiments found | Page 1 of 1 |

Nr.	Hypothesis	Title	Submitter			
1	testExp	testExp	Juergen Hartler			

1 Experiments found | Page 1 of 1 |

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.



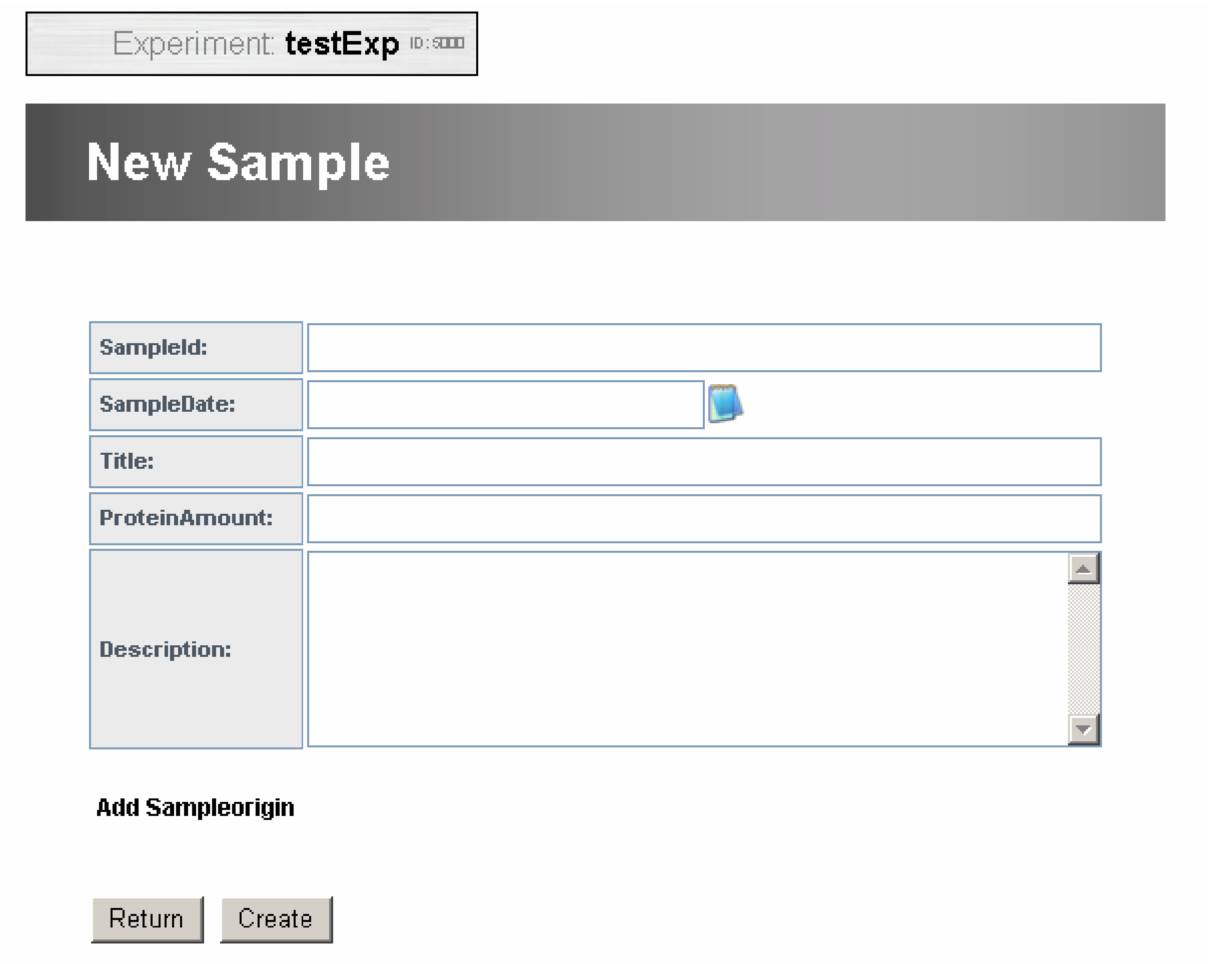
2 Samples found | Page 1 of 1 |

Nr.	SampleId	SampleDate	Title	Description	ProteinAmount			
1	forLexi	2005-07-05	forLexi					✕
2	newMascot	2005-08-04	newMascot					✕

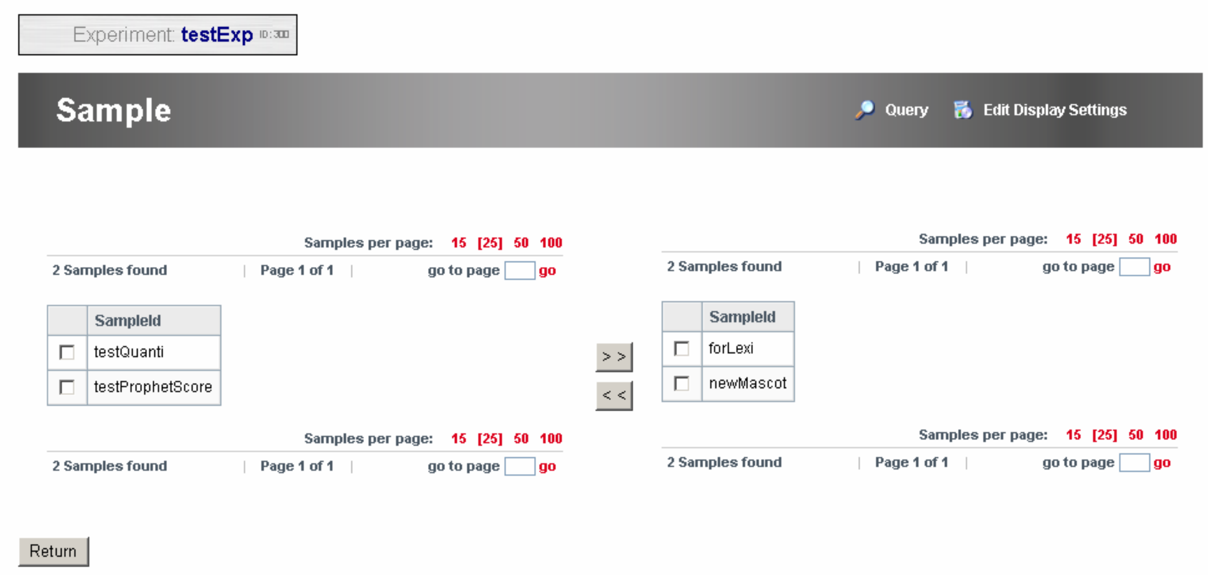
2 Samples found | Page 1 of 1 |

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.



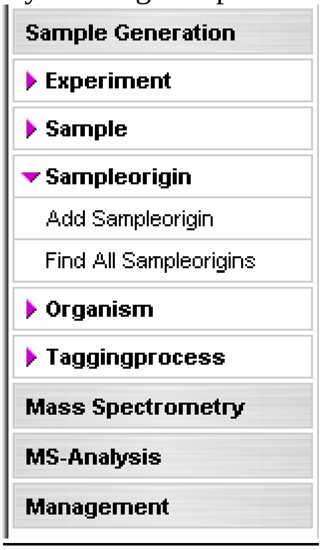
When you use the “Add Samples” button you can add or remove existing samples to or from your experiment.



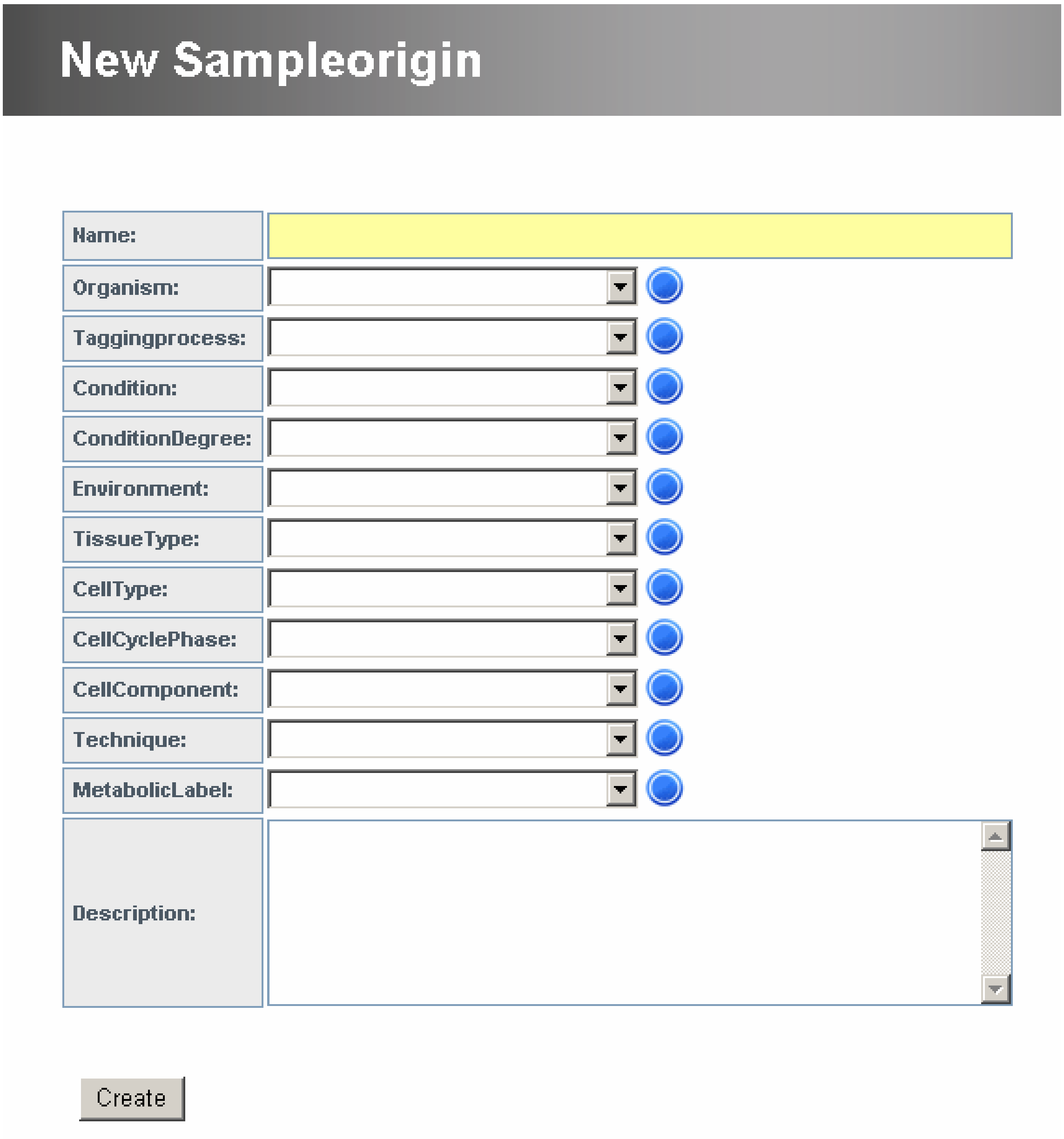
On the left side the addable samples are listed and on the right side the already added samples are listed. The left side is completely queryable. When you want to add samples you simply check the desired checkboxes of the samples on the left side and push the “>>” button. When you want to remove samples 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.

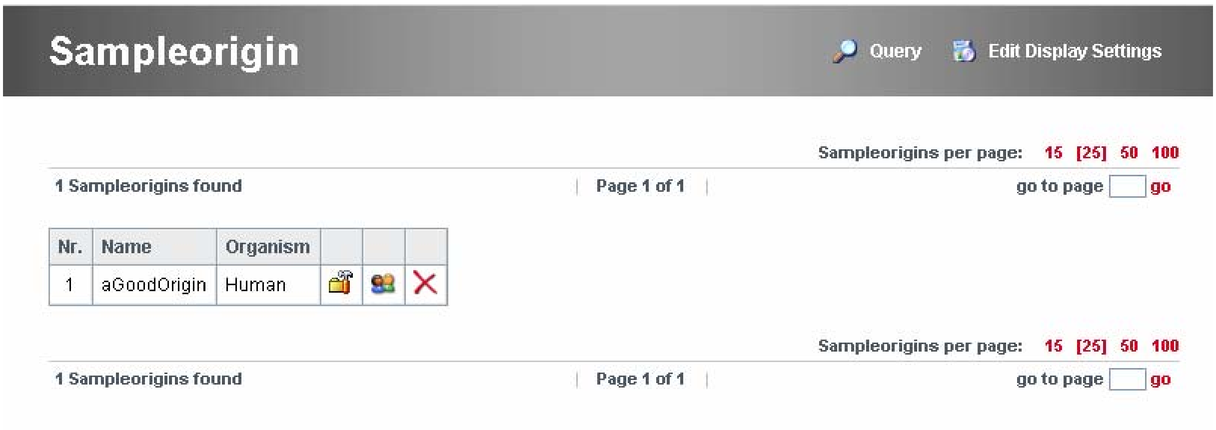


With the “Add Samplorigin” you can add new sample origins.



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”.

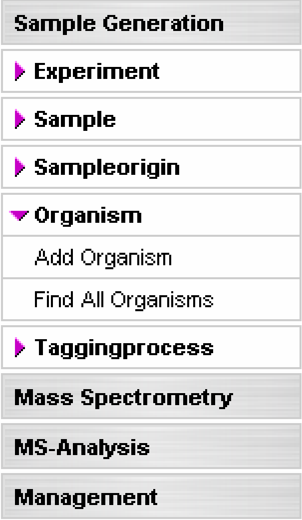
With a click on the button “Find All Sampleorigins” you get an overview of all your sample origins:



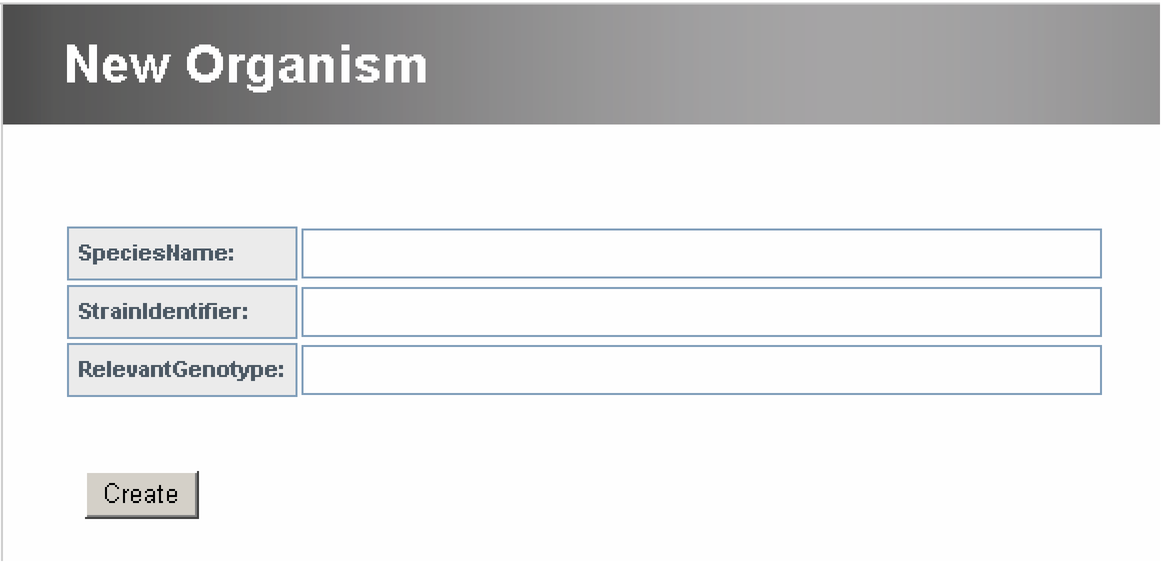
Nr.	Name	Organism			
1	aGoodOrigin	Human			

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:

Organisms per page: 15 [25] 50 100

1 Organisms found | Page 1 of 1 | go to page go

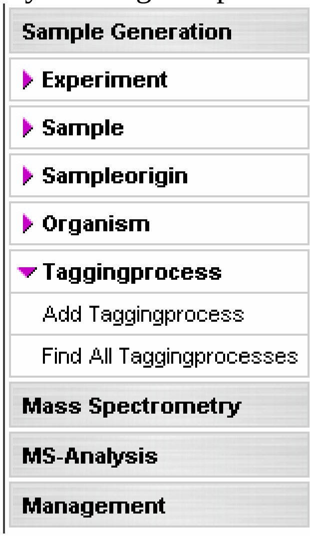
Nr.	SpeciesName			
1	Human			

Organisms per page: 15 [25] 50 100

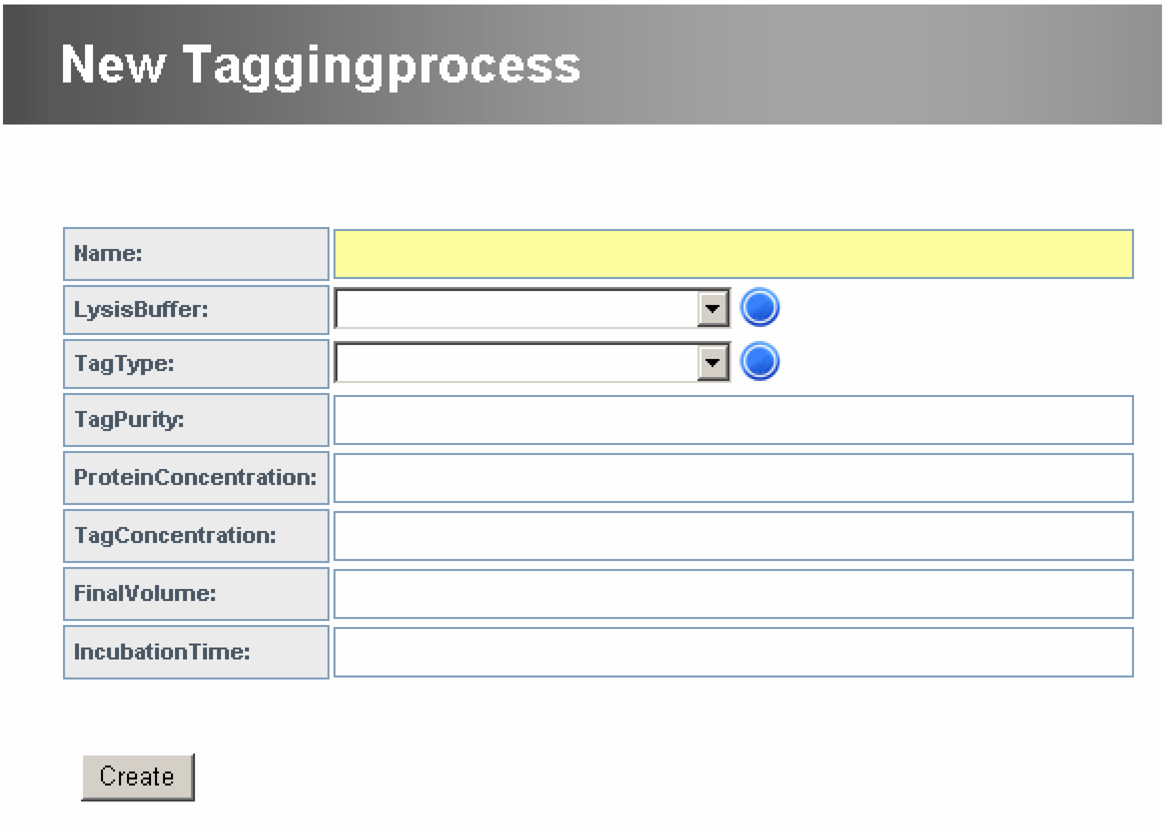
1 Organisms found | Page 1 of 1 | go to page go

3.5 Taggingprocess:

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



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

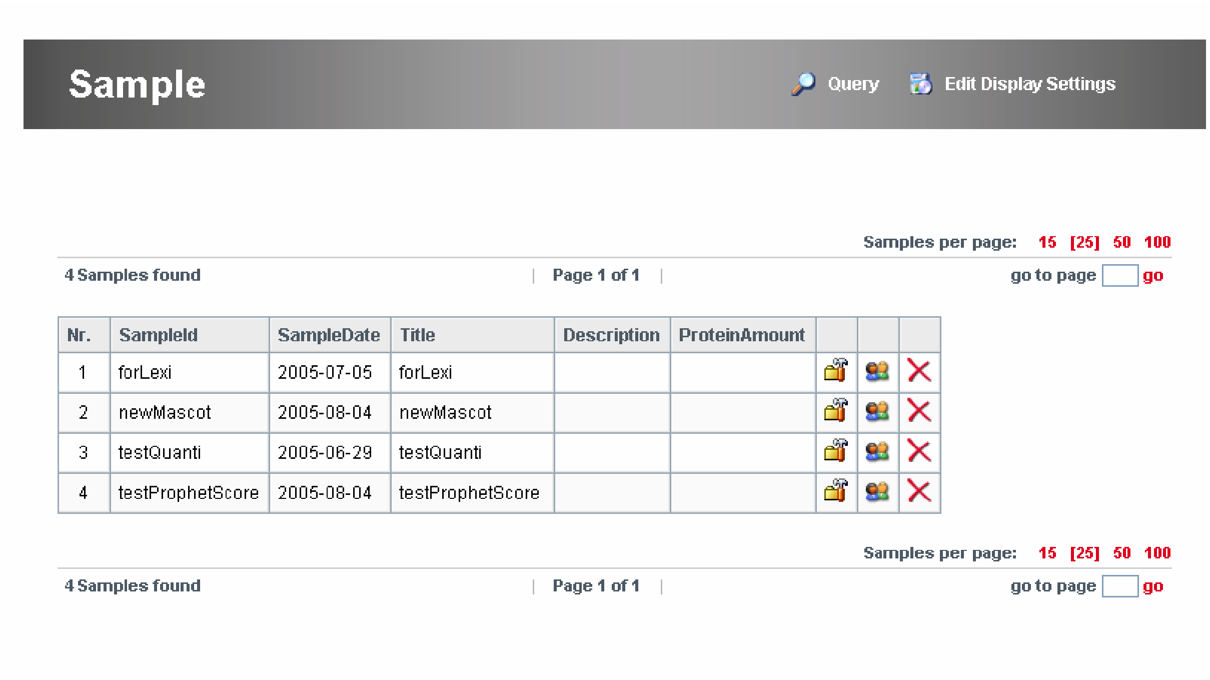


With a click on the button “Find All Taggingprocesses“ you get an overview of all your tagging processes:

Nr.	Name			
1	myTaggingProcess			✕

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:

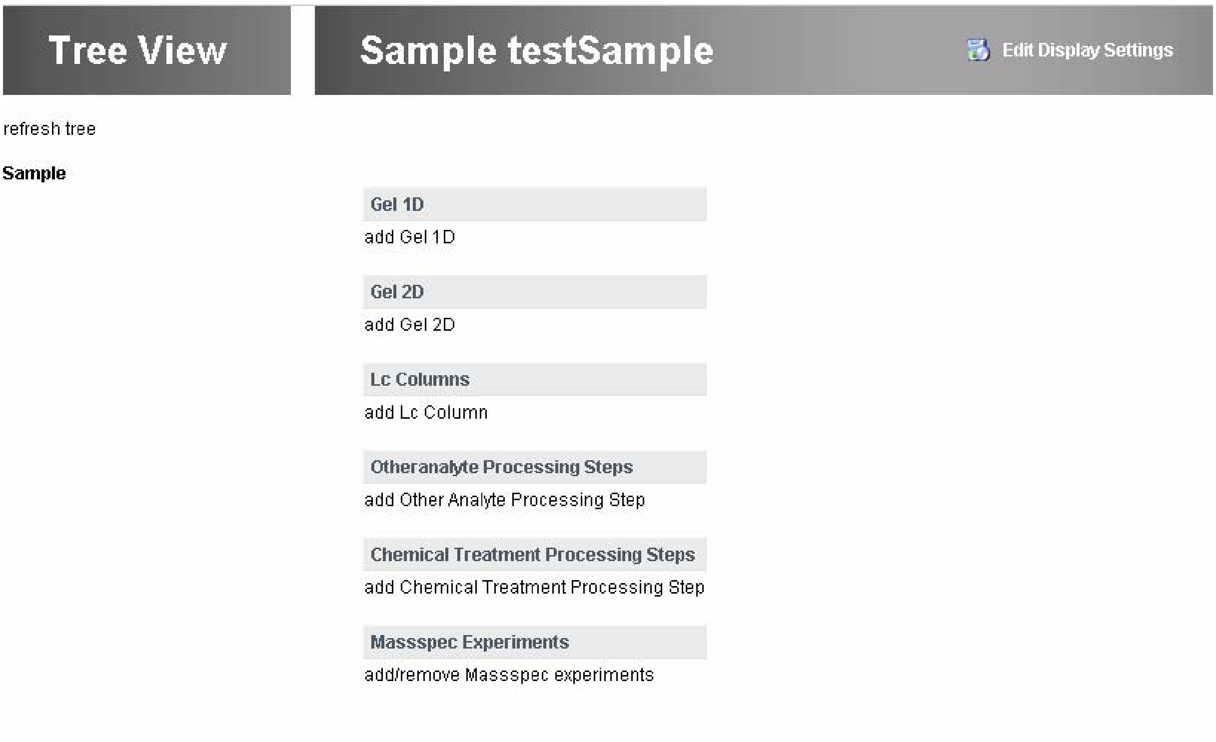


4 Samples found | Page 1 of 1 |

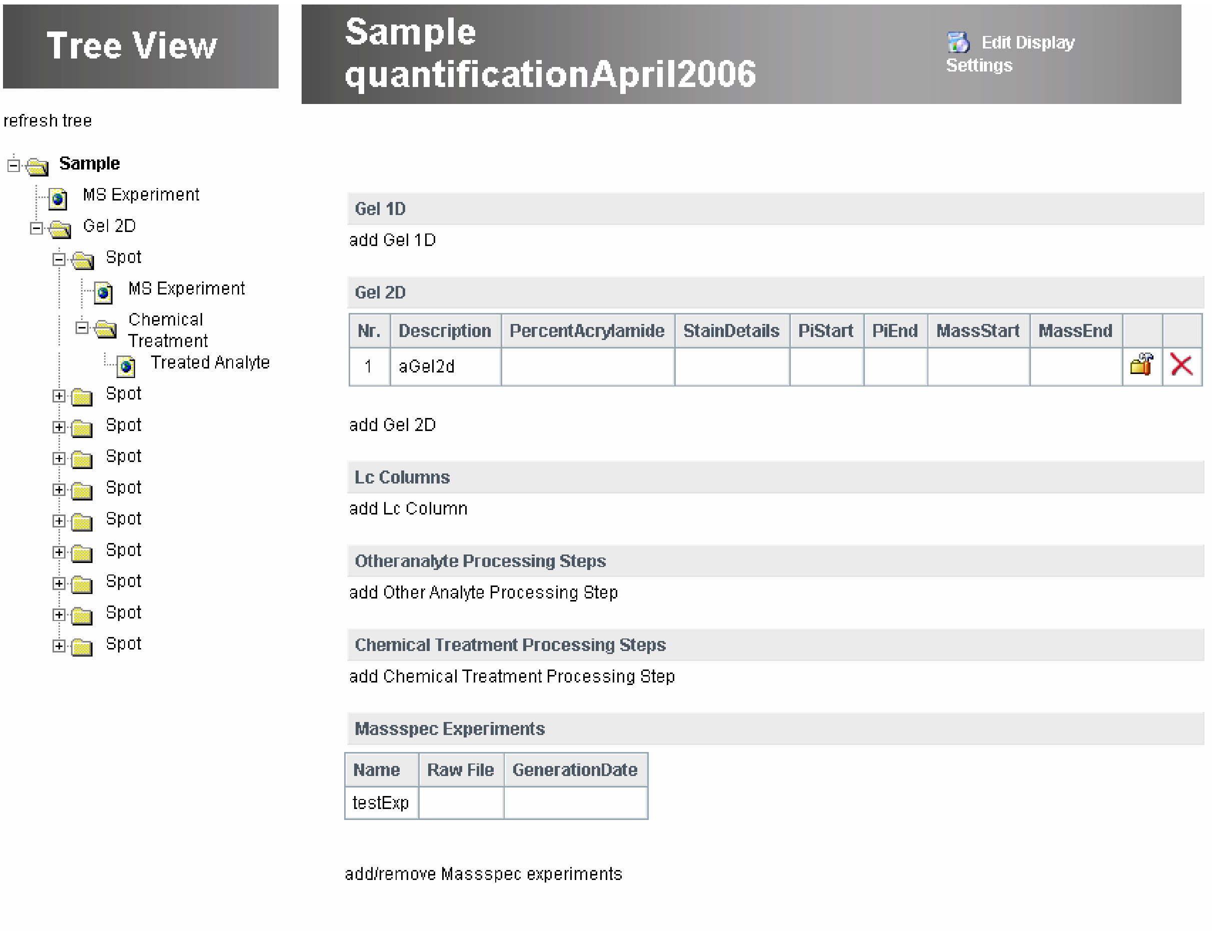
Nr.	SampleId	SampleDate	Title	Description	ProteinAmount			
1	forLexi	2005-07-05	forLexi					✕
2	newMascot	2005-08-04	newMascot					✕
3	testQuanti	2005-06-29	testQuanti					✕
4	testProphetScore	2005-08-04	testProphetScore					✕

4 Samples found | Page 1 of 1 |

When you click on the name for “sampleId” in the corresponding column you want to get more information 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:



Sample quantificationApril2006

- Sample
  - MS Experiment
  - Gel 2D
    - Spot
      - MS Experiment
      - Chemical Treatment
        - Treated Analyte
    - Spot
    - Spot
    - Spot
    - Spot
    - Spot
    - Spot
    - Spot
    - Spot
    - Spot

Gel 1D

add Gel 1D

Gel 2D

Nr.	Description	PercentAcrylamide	StainDetails	PiStart	PiEnd	MassStart	MassEnd		
1	aGel2d								✗

add Gel 2D

Lc Columns

add Lc Column

Otheranalyte Processing Steps

add Other Analyte Processing Step

Chemical Treatment Processing Steps

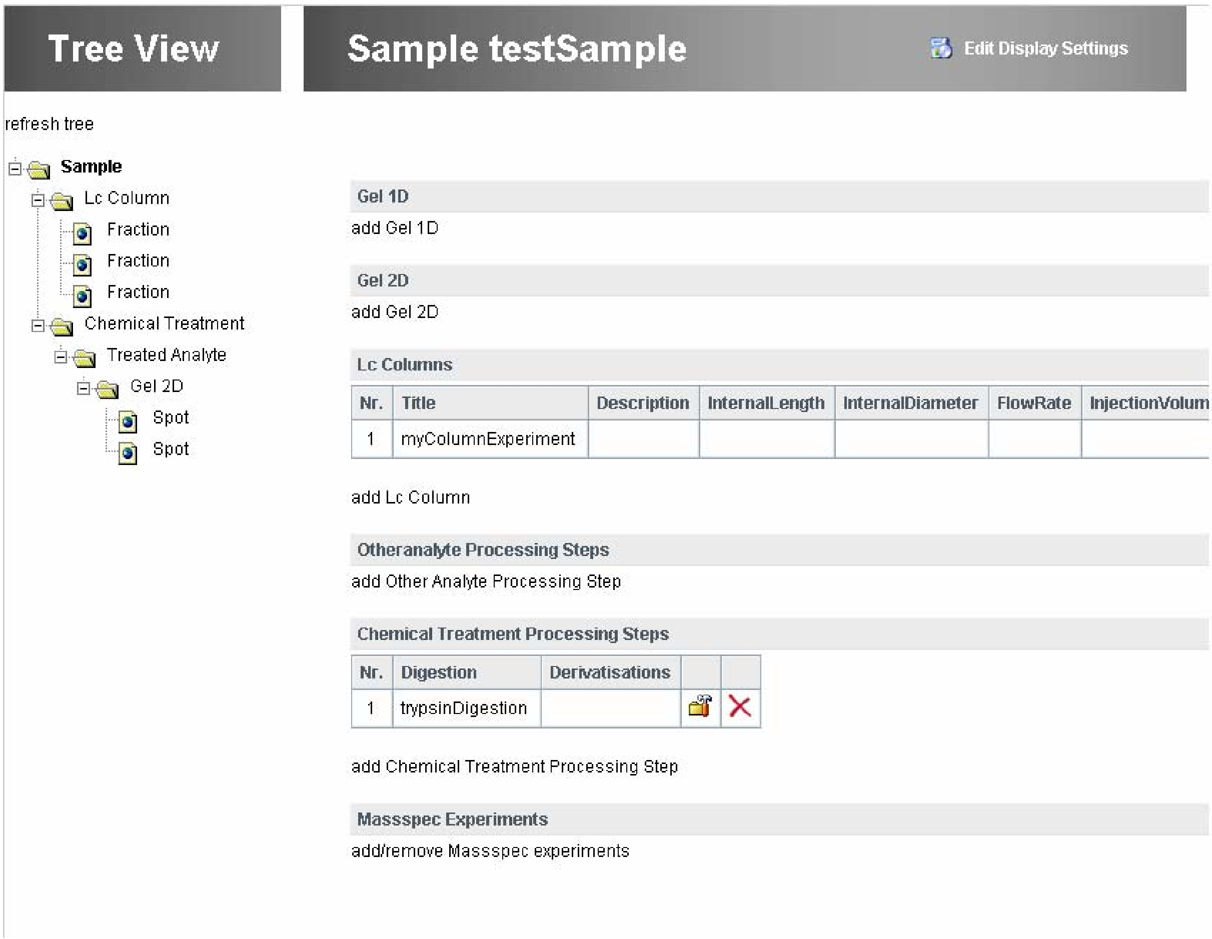
add Chemical Treatment Processing Step

Massspec Experiments

Name	Raw File	GenerationDate
testExp		

add/remove Massspec experiments

The page split 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 run it over an LC-Column, and you got 3 Fraction which are interesting, and the other half was first digested with trypsin, you got one treated analyte, and with this one you made a 2D-Gel where you got a 2 interesting spots. Than the tree would look like the following:



- Sample
  - Lc Column
    - Fraction
    - Fraction
    - Fraction
  - Chemical Treatment
    - Treated Analyte
      - Gel 2D
        - Spot
        - Spot

Sample testSample

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

Nr.	Title	Description	InternalLength	InternalDiameter	FlowRate	InjectionVolum
1	myColumnExperiment					

add Lc Column

Otheranalyte Processing Steps

add Other Analyte Processing Step

Chemical Treatment Processing Steps

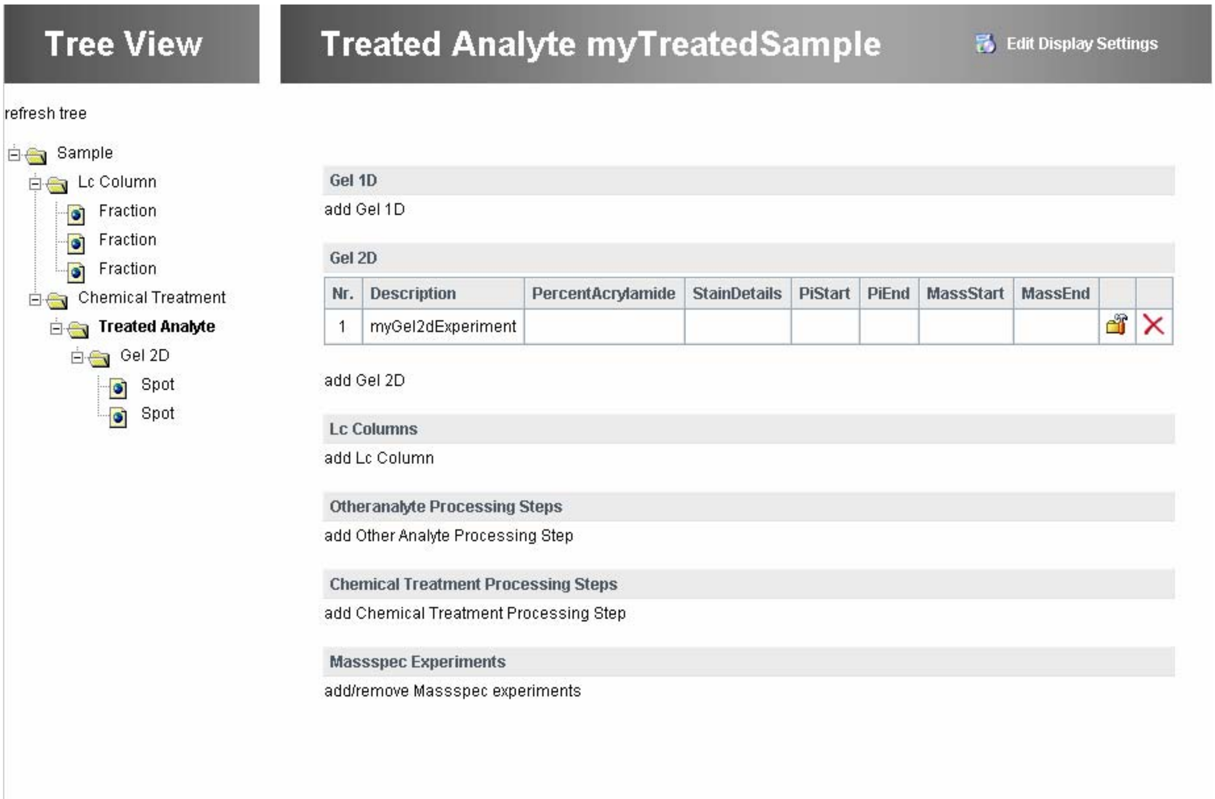
Nr.	Digestion	Derivatisations		
1	trypsinDigestion			✗

add Chemical Treatment Processing Step

Massspec Experiments

add/remove Massspec experiments

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. When you 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:

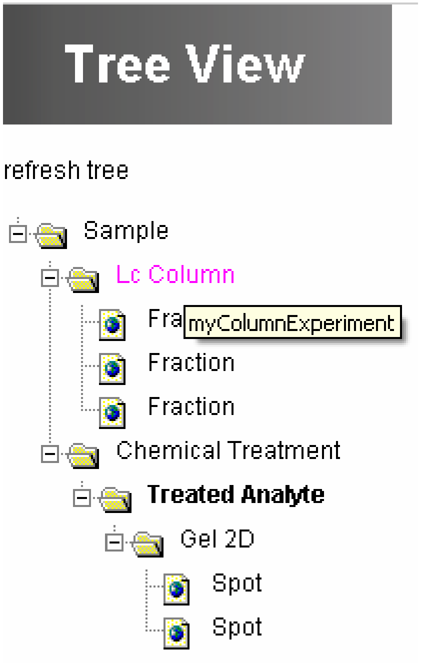


Nr.	Description	PercentAcrylamide	StainDetails	PiStart	PiEnd	MassStart	MassEnd		
1	myGel2dExperiment								

There are 5 different processing methods. A Gel1D leads to band (for detailed information see chapter 4.2 Gel1D), a Gel2D leads to a spot (for detailed information see chapter 4.3 Gel2D), a LC-Column leads to a Fraction (for detailed information see chapter 4.4 LC-Column), a Chemical Treatment leads to a Treated Analyte (for detailed information see chapter 4.5 Chemical Treatment), and a Other Analyte Processing Step (for detailed information see chapter 4.6 Other Analyte Processing Step) leads to an Other Analyte. For all of the analytes Massspec experiments can be add (for detailed information about the adding see chapter 4.7 “Adding of Massspec experiments”). How you generate an 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 itself always the types of the analyte processing steps and the analytes are displayed. When you want to know the name of the element you have to hover your mouse over the element a tool tip with the name will appear.



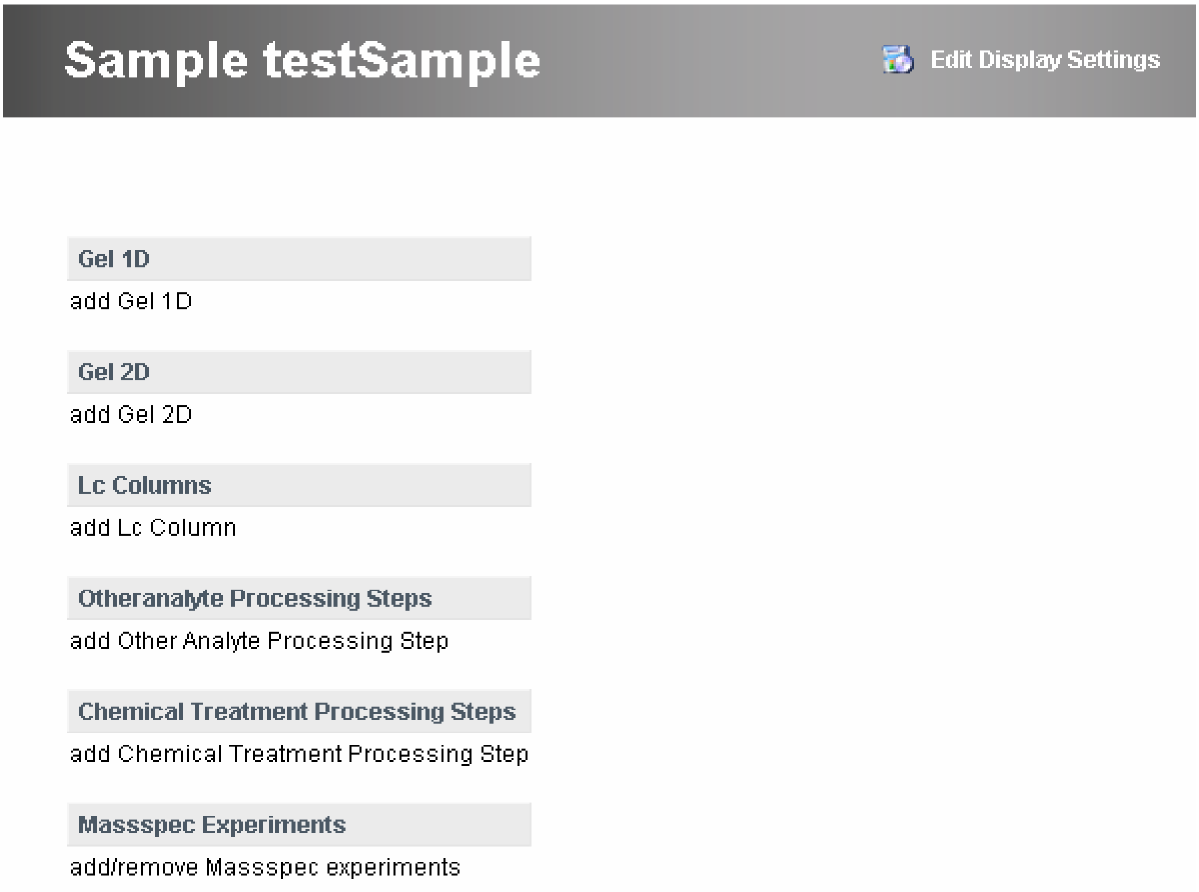
Tree View

refresh tree

- Sample
  - Lc Column
    - Fra myColumnExperiment
    - Fraction
    - Fraction
  - Chemical Treatment
    - **Treated Analyte**
      - Gel 2D
        - Spot
        - Spot

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. For an update press the refresh tree.

4.2 Gel1D:



Sample testSample

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Otheranalyte Processing Steps

add Other Analyte Processing Step

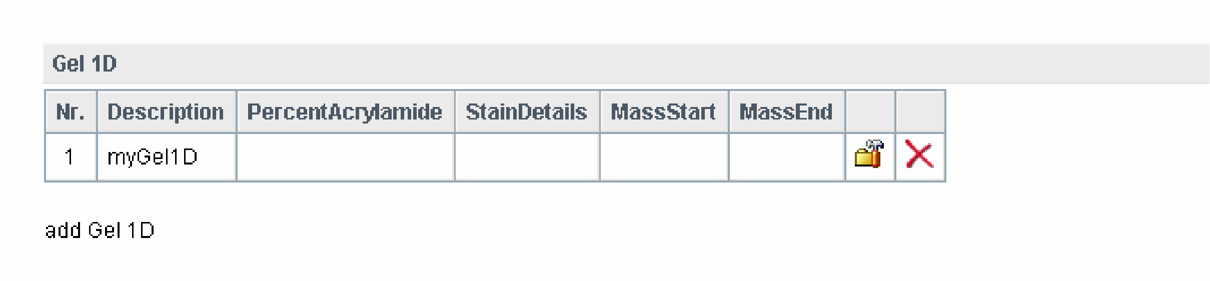
Chemical Treatment Processing Steps

add Chemical Treatment Processing Step

Massspec Experiments

add/remove Massspec experiments

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

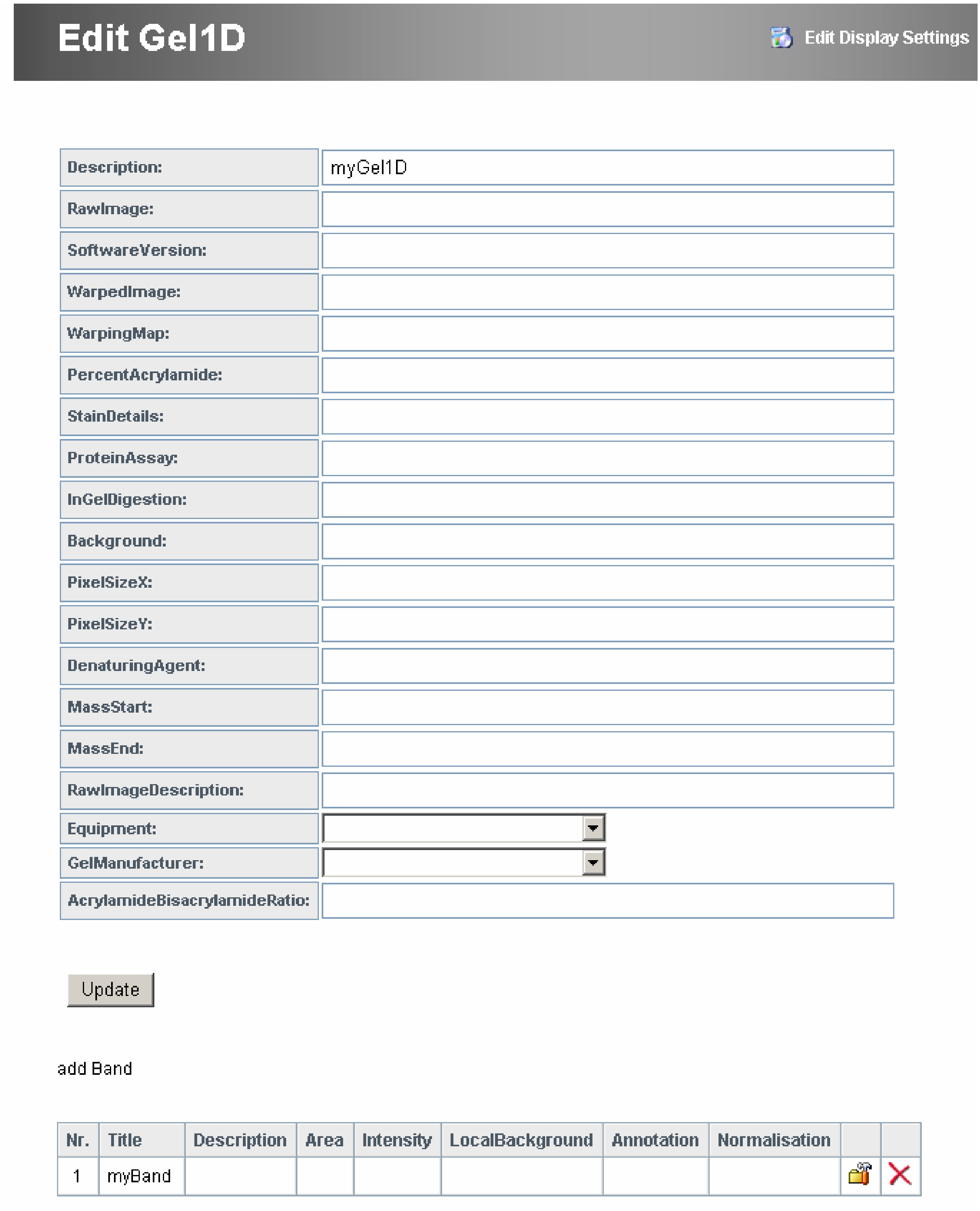


Gel 1D

Nr.	Description	PercentAcrylamide	StainDetails	MassStart	MassEnd		
1	myGel1D					✎	✗

add Gel 1D

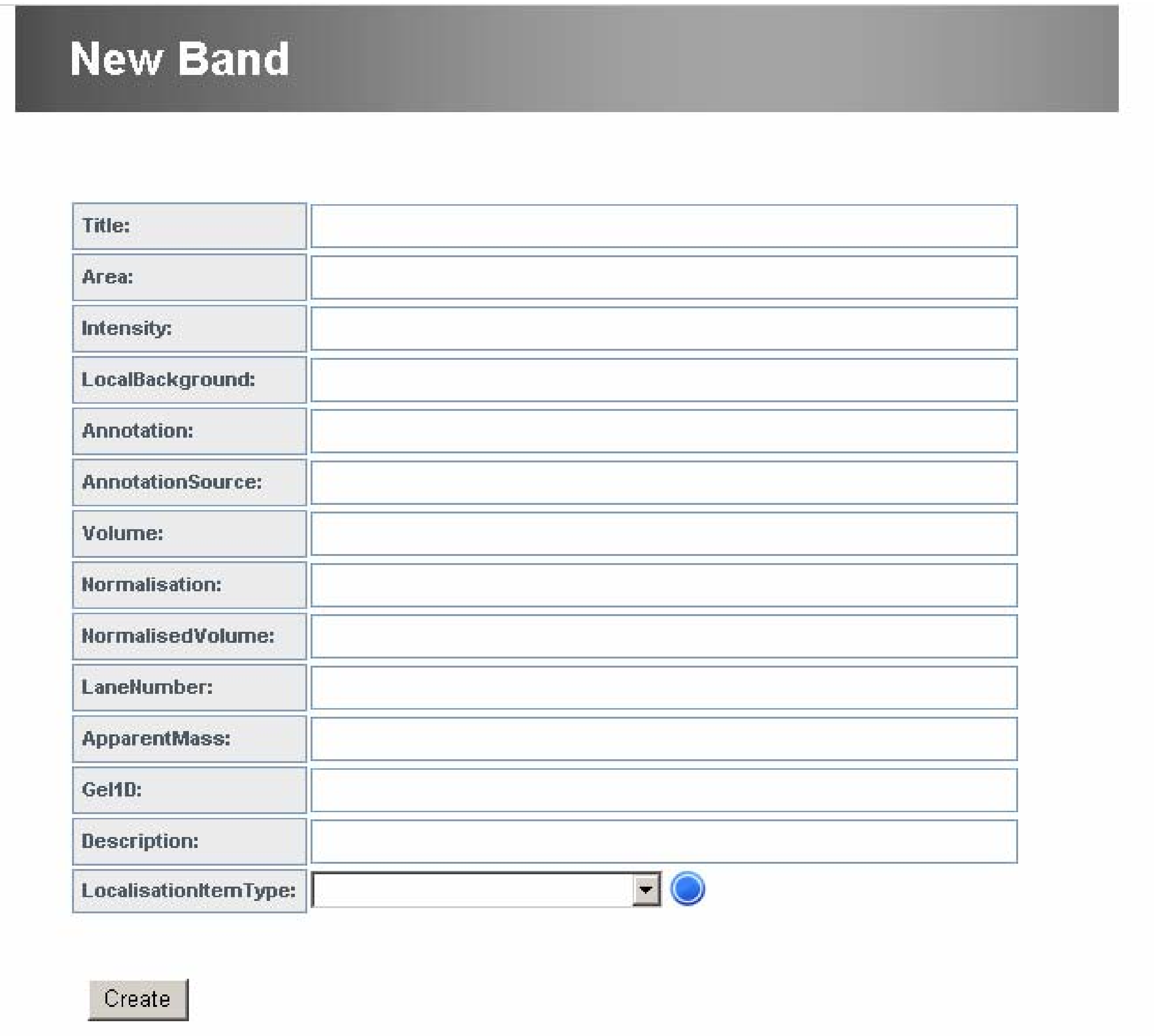
When you click on the description name or on the edit button you will be directed to same page like the create page again.



Description:	myGel1D
RawImage:	
SoftwareVersion:	
WarpedImage:	
WarpingMap:	
PercentAcrylamide:	
StainDetails:	
ProteinAssay:	
InGelDigestion:	
Background:	
PixelSizeX:	
PixelSizeY:	
DenaturingAgent:	
MassStart:	
MassEnd:	
RawImageDescription:	
Equipment:	
GelManufacturer:	
AcrylamideBisacrylamideRatio:	

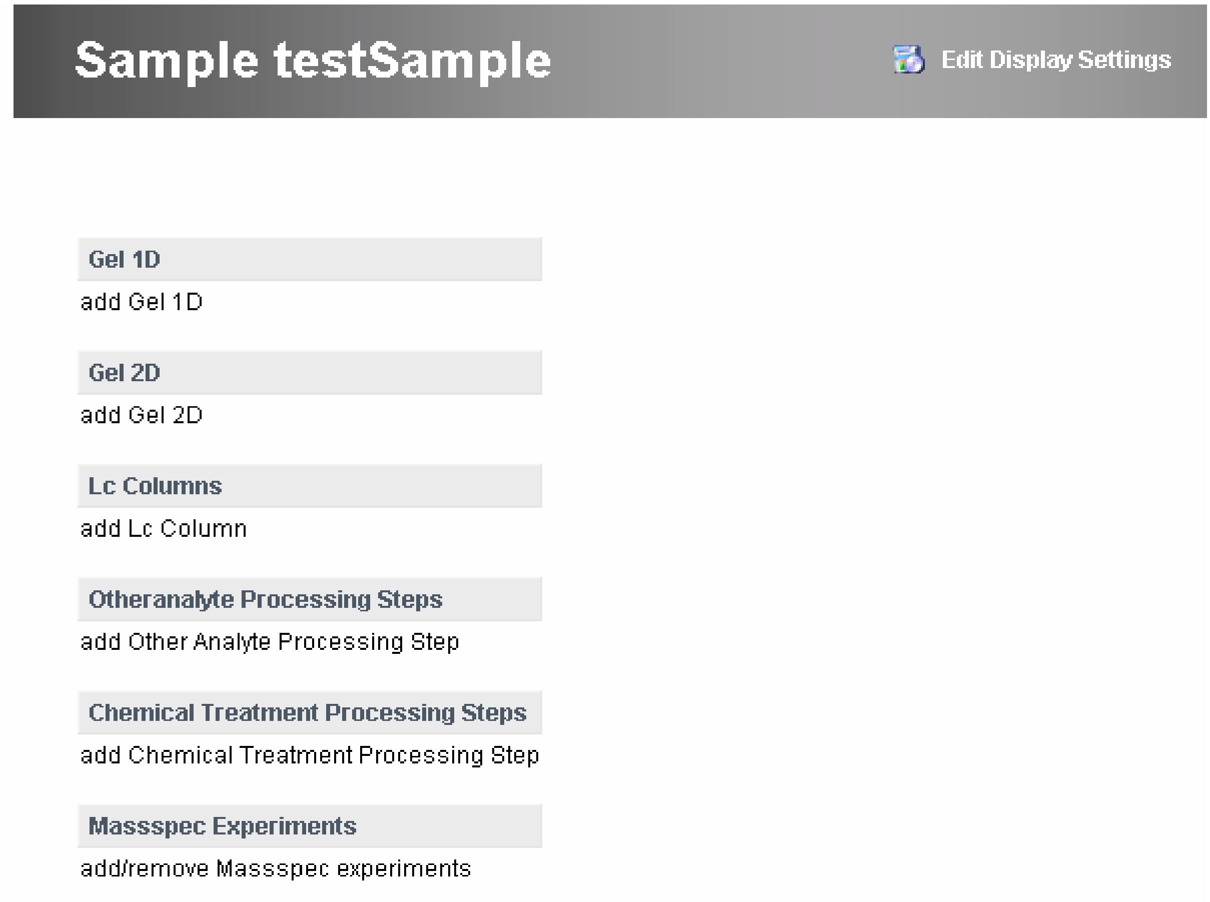
Nr.	Title	Description	Area	Intensity	LocalBackground	Annotation	Normalisation		
1	myBand								✗

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



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

4.3 Gel2D:



Sample testSample

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Otheranalyte Processing Steps

add Other Analyte Processing Step

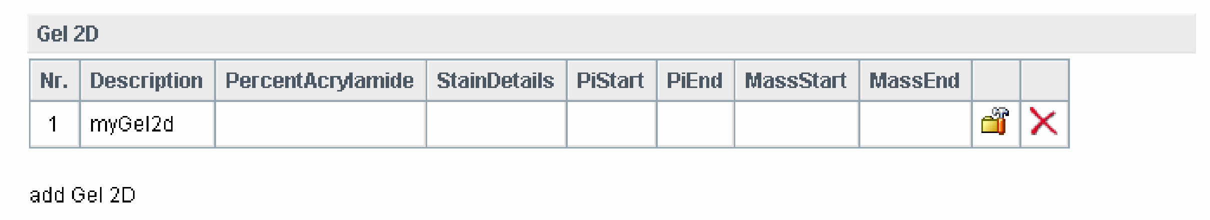
Chemical Treatment Processing Steps

add Chemical Treatment Processing Step

Massspec Experiments

add/remove Massspec experiments

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

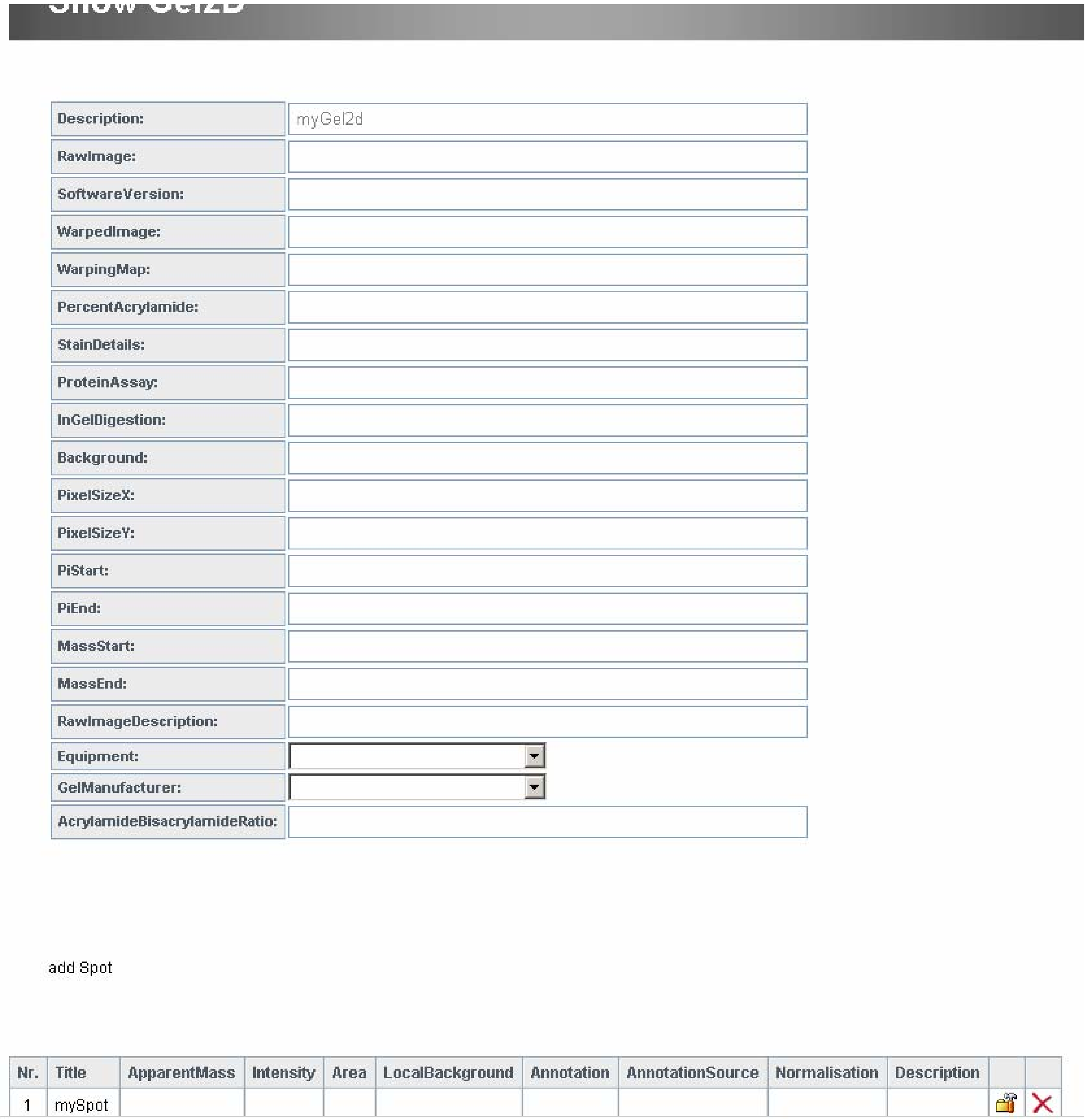


Gel 2D

Nr.	Description	PercentAcrylamide	StainDetails	PiStart	PiEnd	MassStart	MassEnd		
1	myGel2d								✗

add Gel 2D

When you click on the description name or on the edit button you will be directed to same page like the create page again.



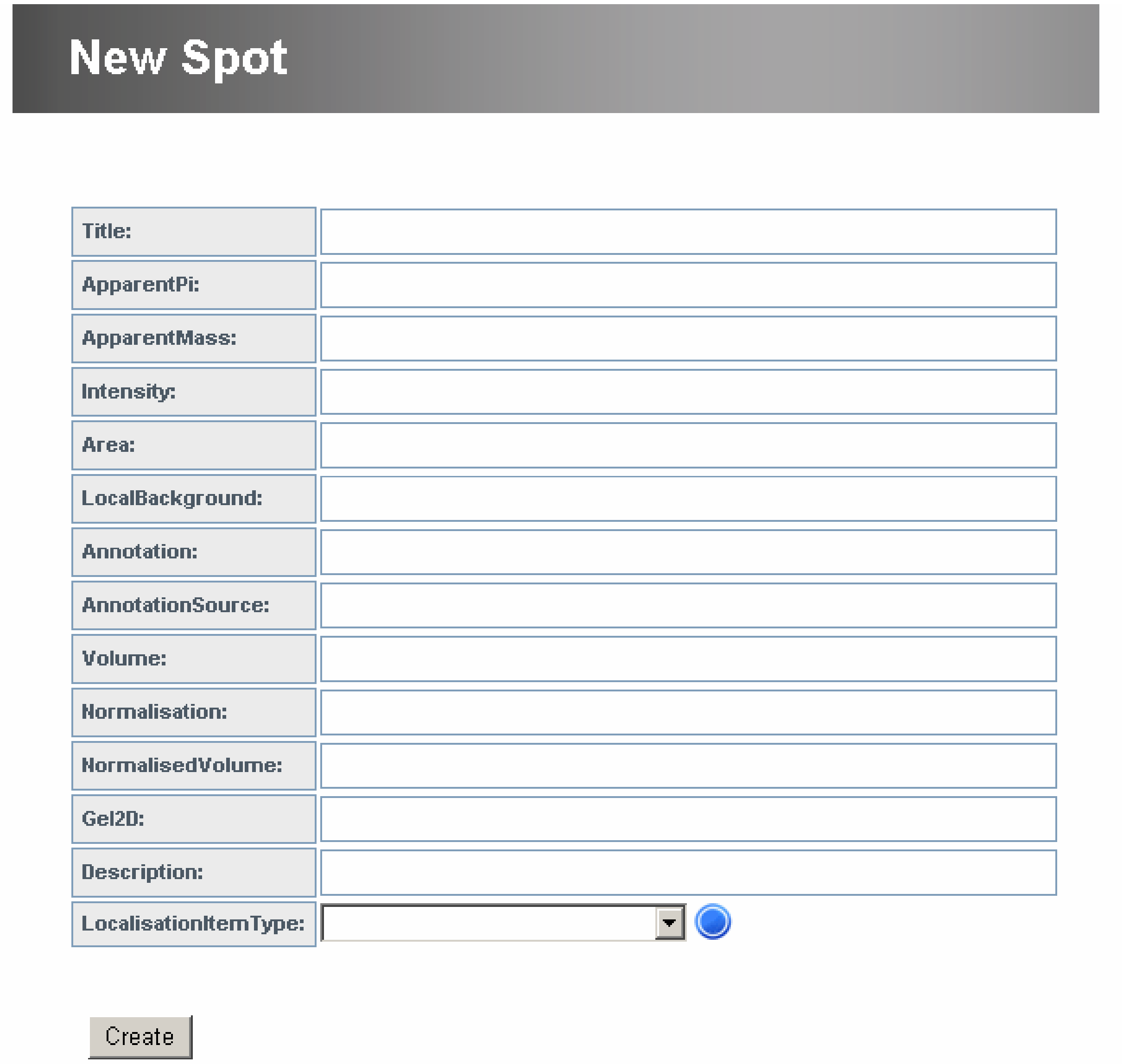
Show Gel2D

Description:	myGel2d
RawImage:	
SoftwareVersion:	
WarpedImage:	
WarpingMap:	
PercentAcrylamide:	
StainDetails:	
ProteinAssay:	
InGelDigestion:	
Background:	
PixelSizeX:	
PixelSizeY:	
PiStart:	
PiEnd:	
MassStart:	
MassEnd:	
RawImageDescription:	
Equipment:	
GelManufacturer:	
AcrylamideBisacrylamideRatio:	

add Spot

Nr.	Title	ApparentMass	Intensity	Area	LocalBackground	Annotation	AnnotationSource	Normalisation	Description		
1	mySpot									✎	✗

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

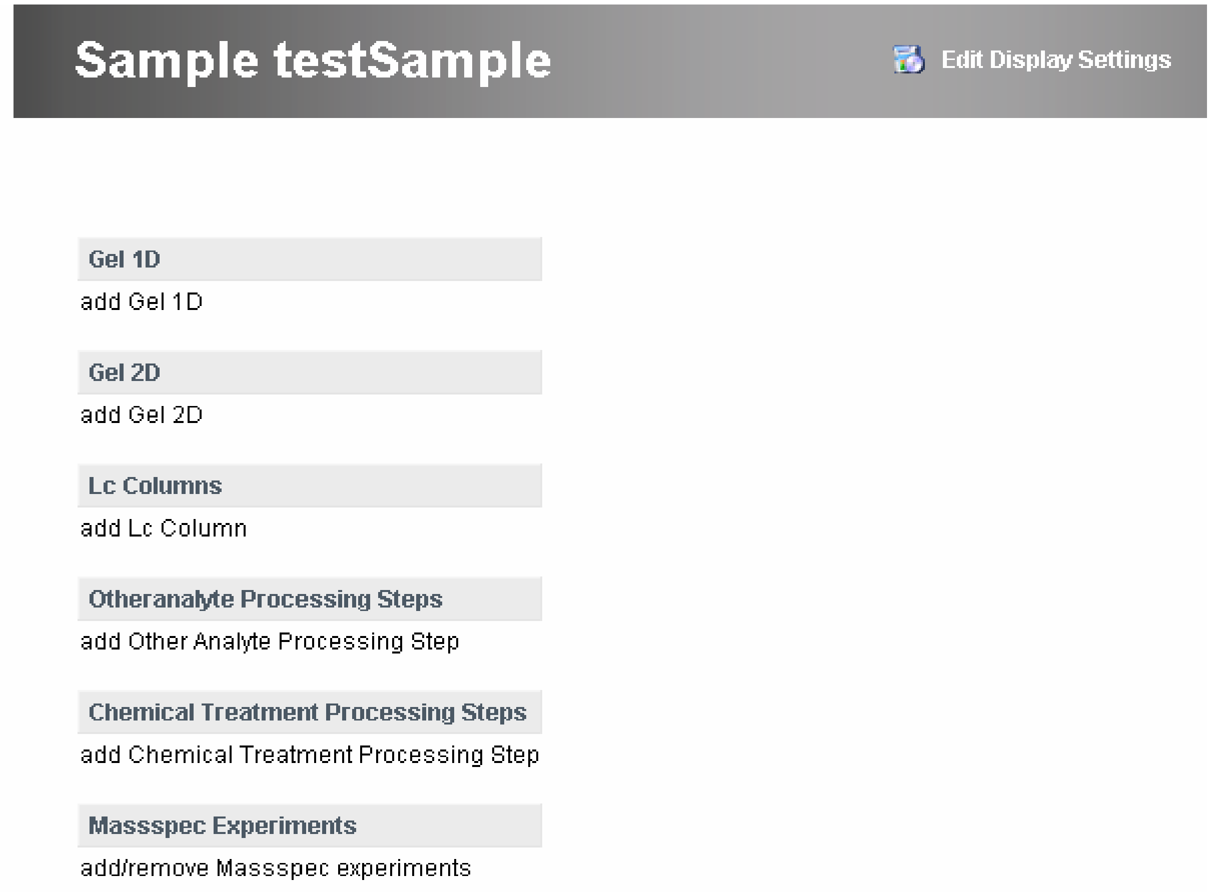


New Spot

Title:	
ApparentPi:	
ApparentMass:	
Intensity:	
Area:	
LocalBackground:	
Annotation:	
AnnotationSource:	
Volume:	
Normalisation:	
NormalisedVolume:	
Gel2D:	
Description:	
LocalisationItemType:	

When you click in the spot on the edit or delete button you reach this “create” page again and you can make your changes, but when click 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.

4.4 LC-Column:



Sample testSample

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Otheranalyte Processing Steps

add Other Analyte Processing Step

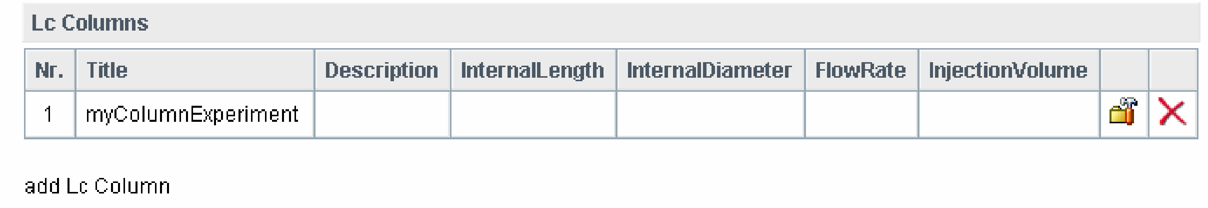
Chemical Treatment Processing Steps

add Chemical Treatment Processing Step

Massspec Experiments

add/remove Massspec experiments

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

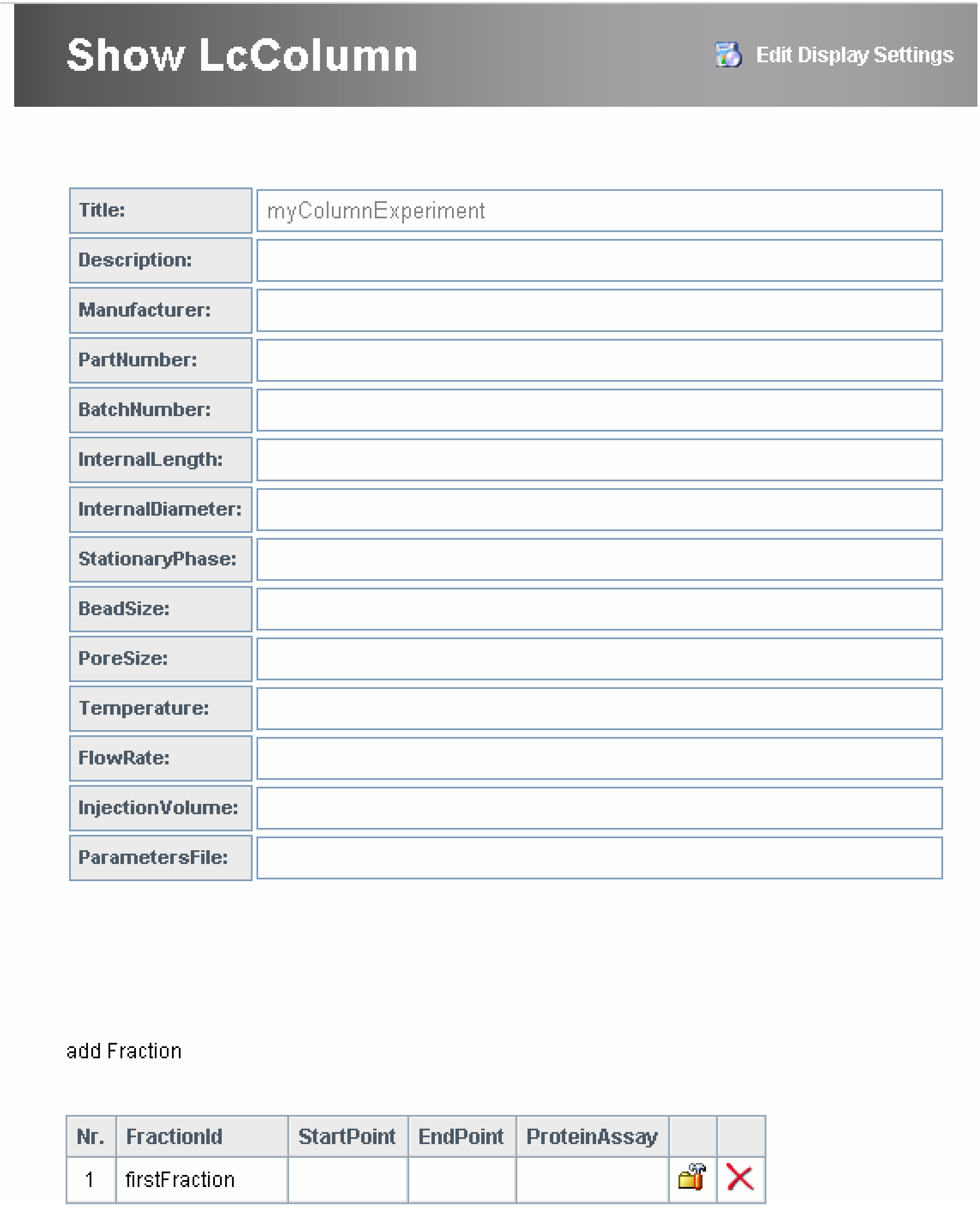


Lc Columns

Nr.	Title	Description	InternalLength	InternalDiameter	FlowRate	InjectionVolume		
1	myColumnExperiment						✎	✕

add Lc Column

When you click on the title name or on the edit button you will be directed to same page like the create page again.



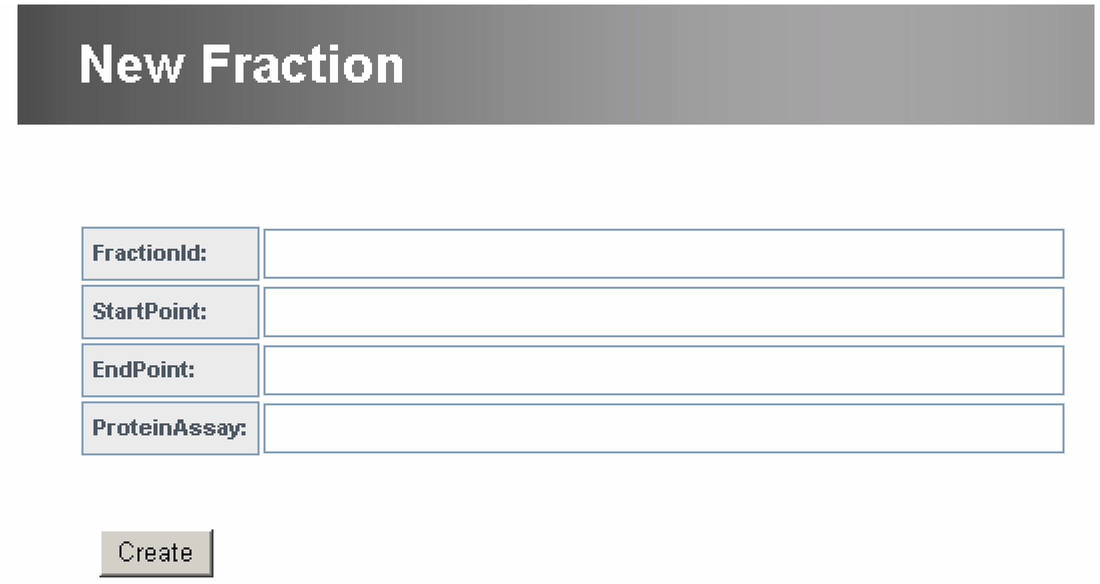
Show LcColumn

Title:	myColumnExperiment
Description:	
Manufacturer:	
PartNumber:	
BatchNumber:	
InternalLength:	
InternalDiameter:	
StationaryPhase:	
BeadSize:	
PoreSize:	
Temperature:	
FlowRate:	
InjectionVolume:	
ParametersFile:	

add Fraction

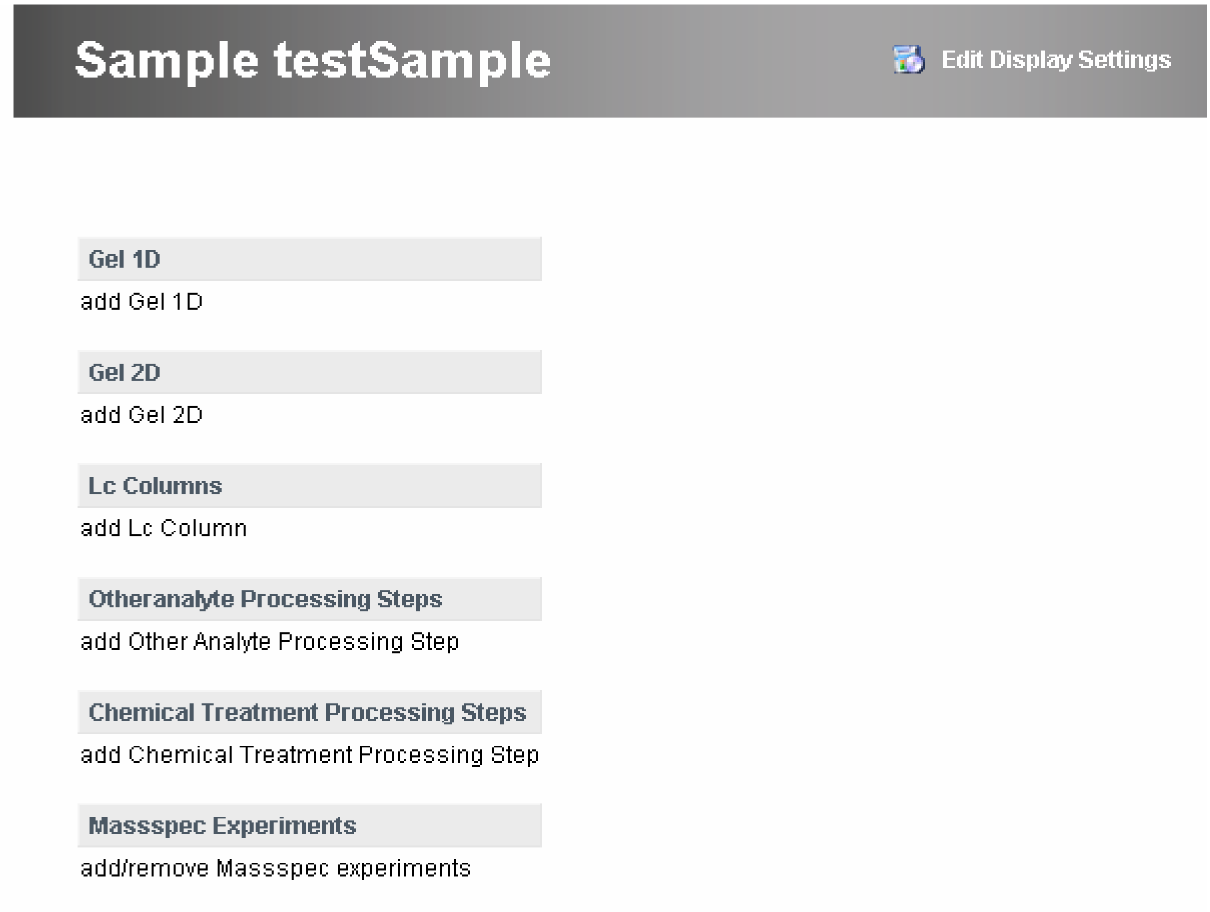
Nr.	FractionId	StartPoint	EndPoint	ProteinAssay		
1	firstFraction					✕

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



When you click in the fraction on the edit or delete button you reach this “create” page again and you can make your changes, but when click 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:

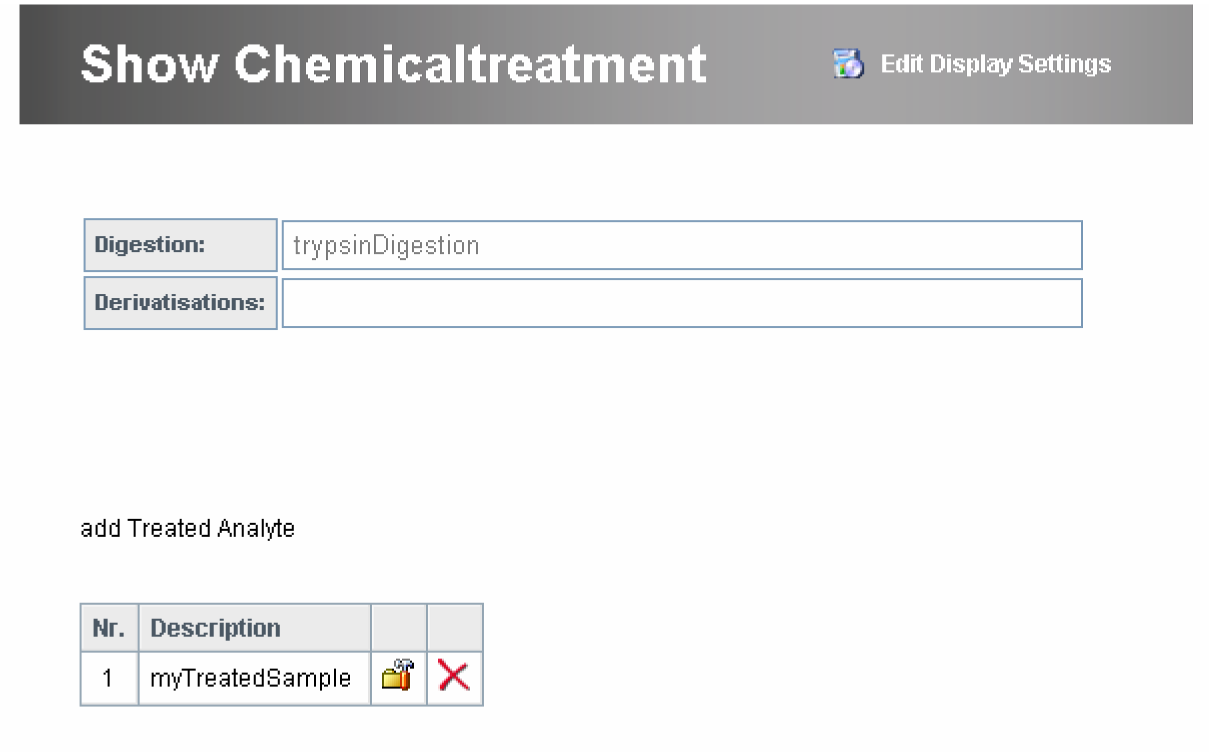


When you are in the page of a sample or an analyte you can add chemical treatmens with the link “add Chemical Treatment Processing Step“. When you added a chemical treatment you will be redirected to the previous page with the added chemical treatment.

Chemical Treatment Processing Steps

Nr.	Digestion	Derivatisations		
1	trypsinDigestion			✕

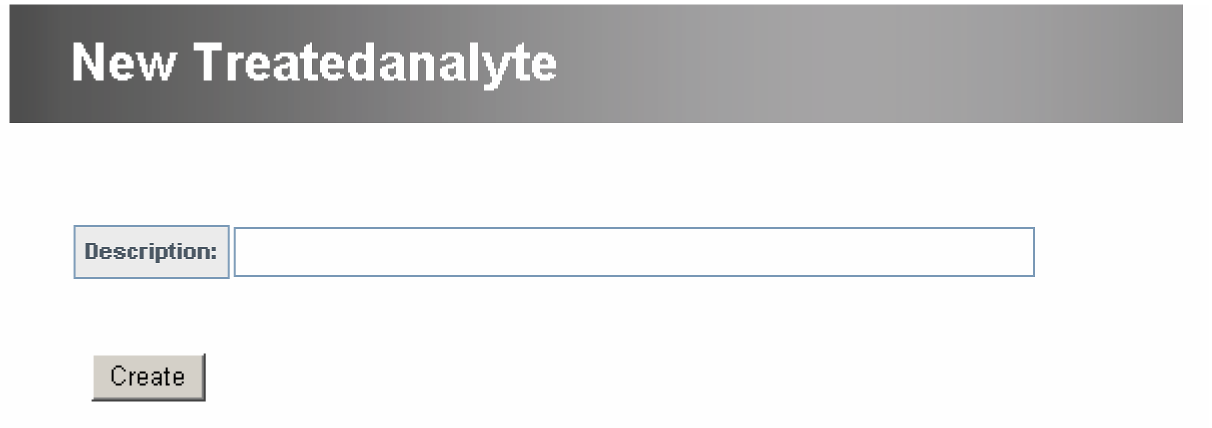
When you click on the digestion name or on the edit button you will be directed to same page like the create page again.



Digestion:	trypsinDigestion
Derivatisations:	

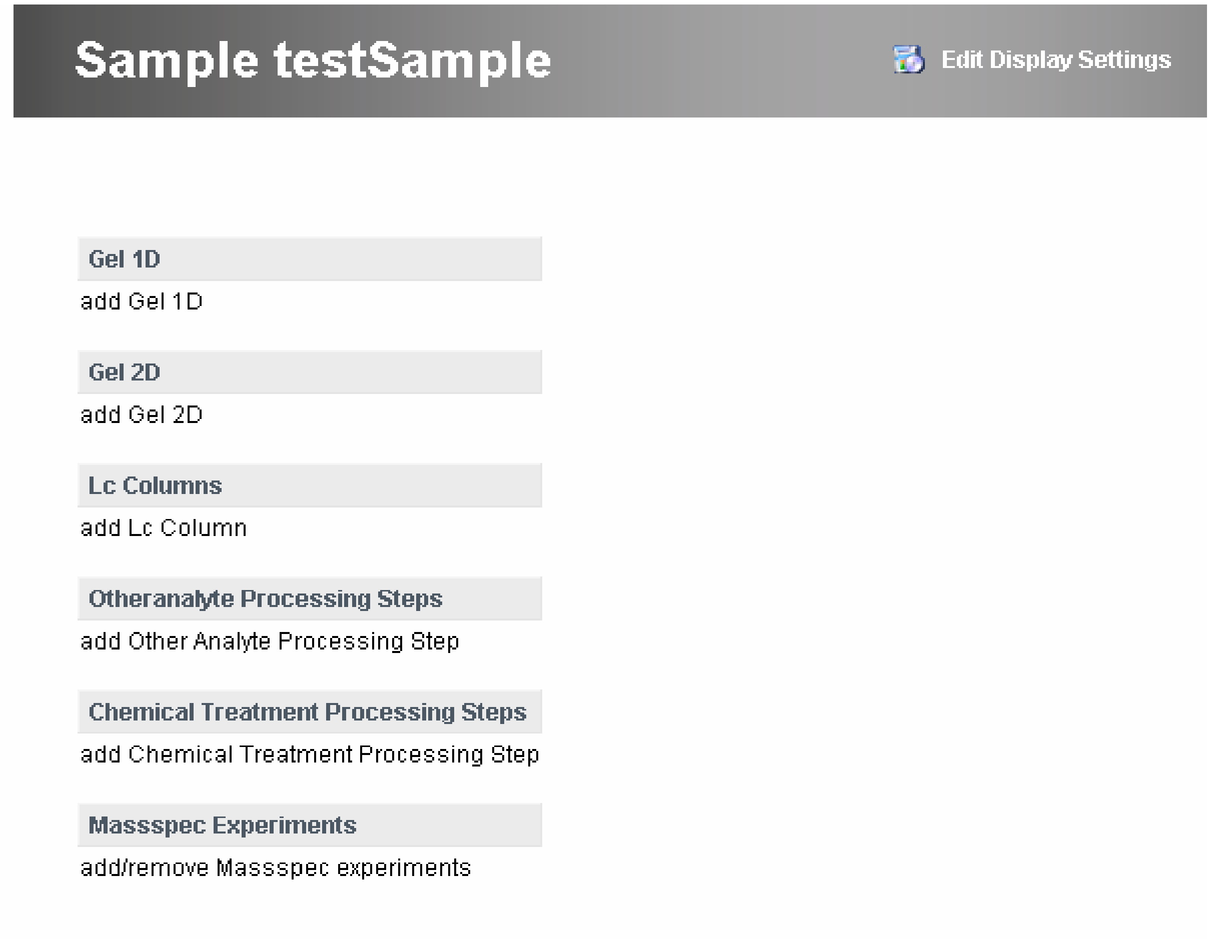
Nr.	Description		
1	myTreatedSample		✕

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



When you click in the treated analyte on the edit or delete button you reach this “create” page again and you can make your changes, but when click 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:



Sample testSample

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Otheranalyte Processing Steps

add Other Analyte Processing Step

Chemical Treatment Processing Steps

add Chemical Treatment Processing Step

Massspec Experiments

add/remove Massspec experiments

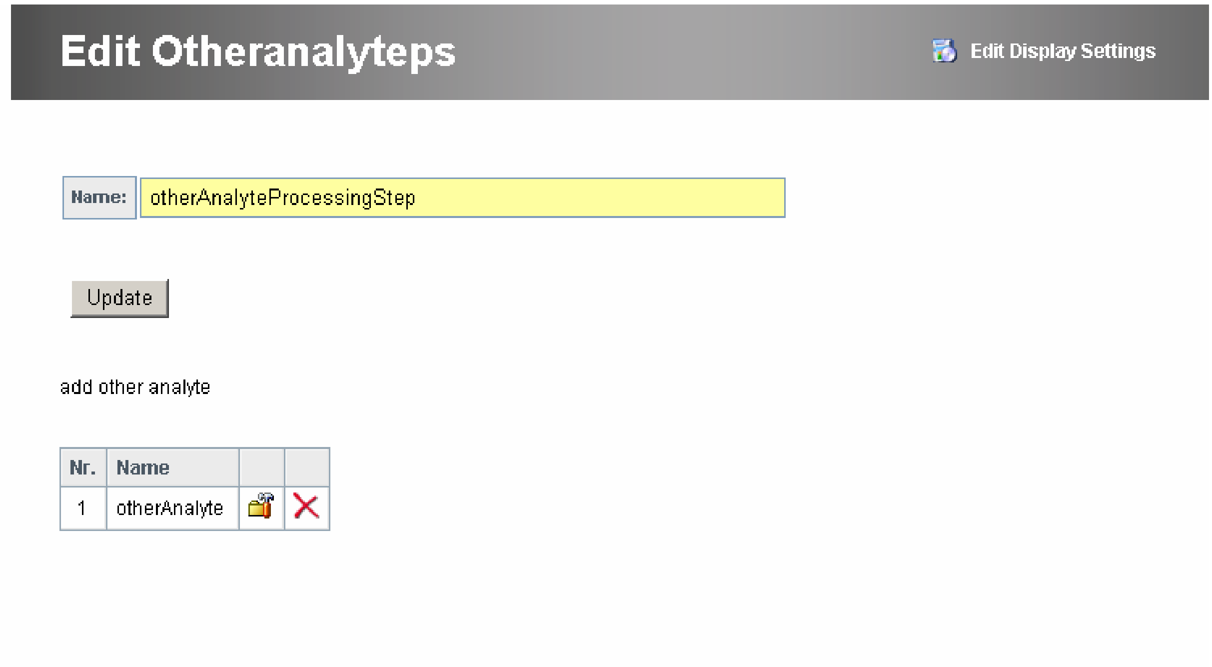
When you are in the page of a sample or an analyte you can add other analyte processing steps with the link “add Other Analyte Processing Step“. When you added an other analyte processing step you will be redirected to the previous page with the added other analyte processing step.

Otheranalyte Processing Steps

Nr.	Name		
1	otherAnalyteProcessingStep	✎	✕

add Other Analyte Processing Step

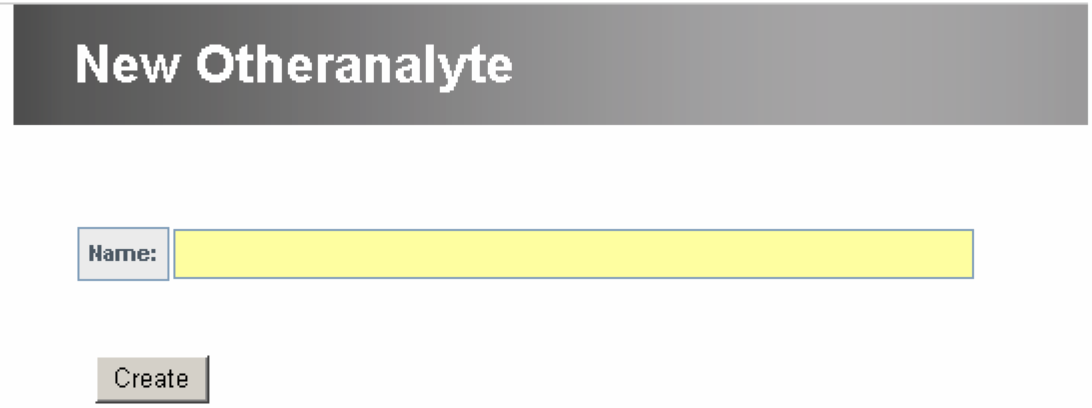
When you click on the name or on the edit button you will be directed to same page like the create page again.



Name: otherAnalyteProcessingStep

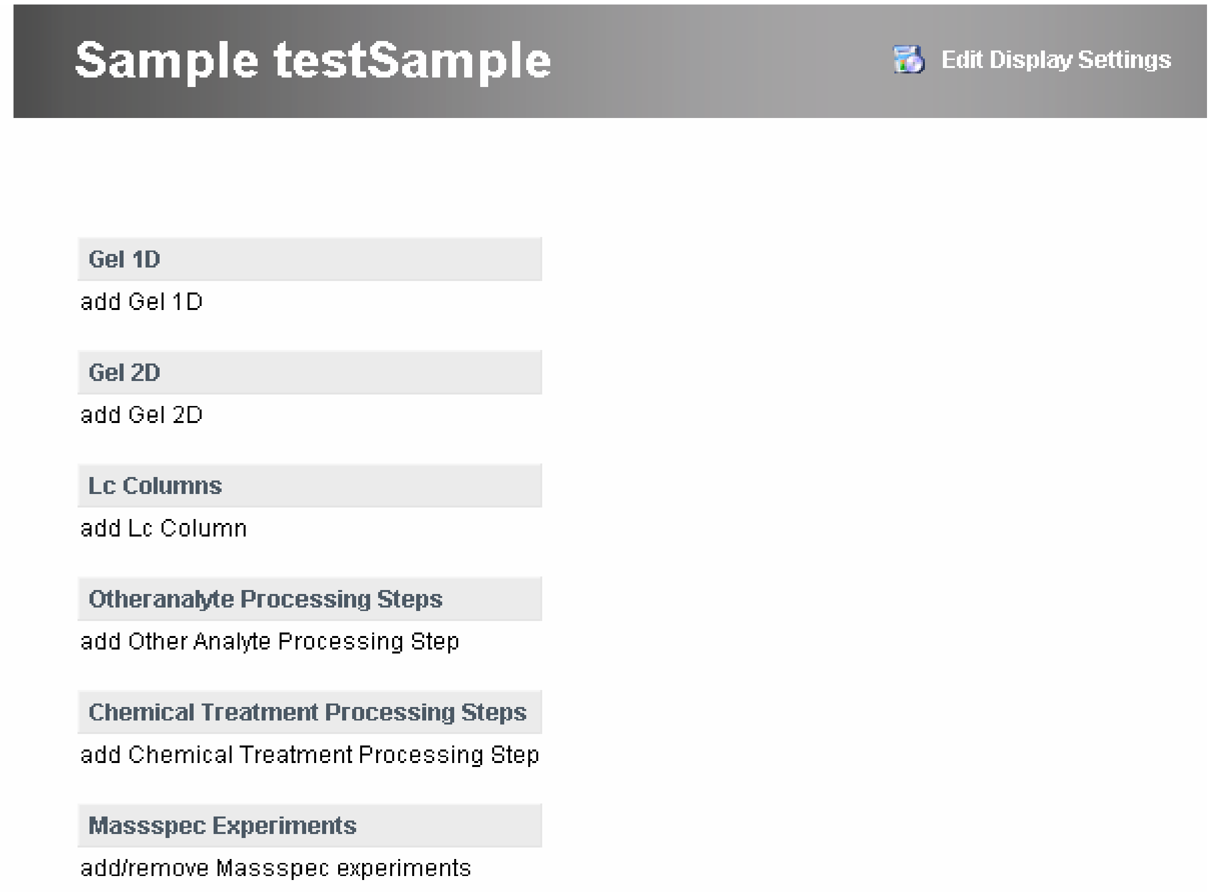
Nr.	Name		
1	otherAnalyte	🔧	✗

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



When you click in the other analyte on the edit or delete button you reach this “create” page again and you can make your changes, but when click 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



Sample testSample

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Otheranalyte Processing Steps

add Other Analyte Processing Step

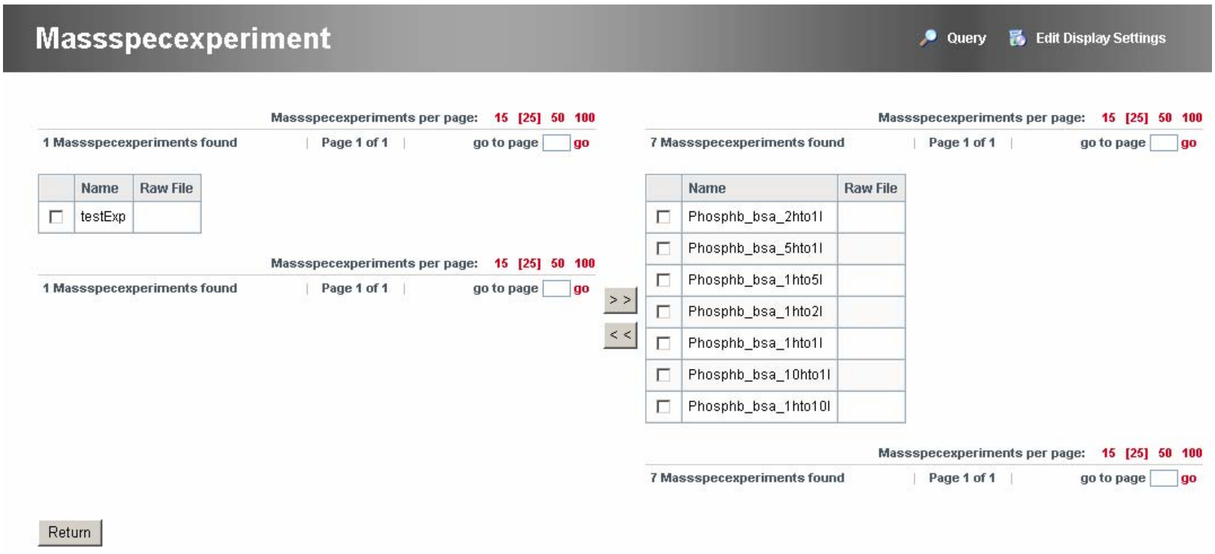
Chemical Treatment Processing Steps

add Chemical Treatment Processing Step

Massspec Experiments

add/remove Massspec experiments

When you 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 in the page of a sample or an analyte you can add other mass spectrometry experiments the link “add/remove Massspec experiments“.



Massspecexperiment

Massspecexperiments per page: 15 [25] 50 100

1 Massspecexperiments found | Page 1 of 1 | go to page go

	Name	Raw File
☐	testExp	

Massspecexperiments per page: 15 [25] 50 100

1 Massspecexperiments found | Page 1 of 1 | go to page go

Massspecexperiments per page: 15 [25] 50 100

7 Massspecexperiments found | Page 1 of 1 | go to page go

	Name	Raw File
☐	Phosphb_bsa_2hto1l	
☐	Phosphb_bsa_5hto1l	
☐	Phosphb_bsa_1hto5l	
☐	Phosphb_bsa_1hto2l	
☐	Phosphb_bsa_1hto1l	
☐	Phosphb_bsa_10hto1l	
☐	Phosphb_bsa_1hto10l	

Massspecexperiments per page: 15 [25] 50 100

7 Massspecexperiments found | Page 1 of 1 | go to page go

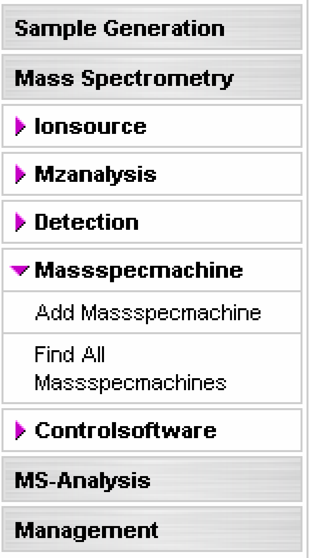
The adding of the massspec experiments to an analyte works the same way like the adding of samples to experiments (see chapter 3.2.2). The only difference is that here are only mass spectrometry experiments are displayed on the left side, which are not already added to an analyte, while the sample can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

5. Mass Spectrometry:

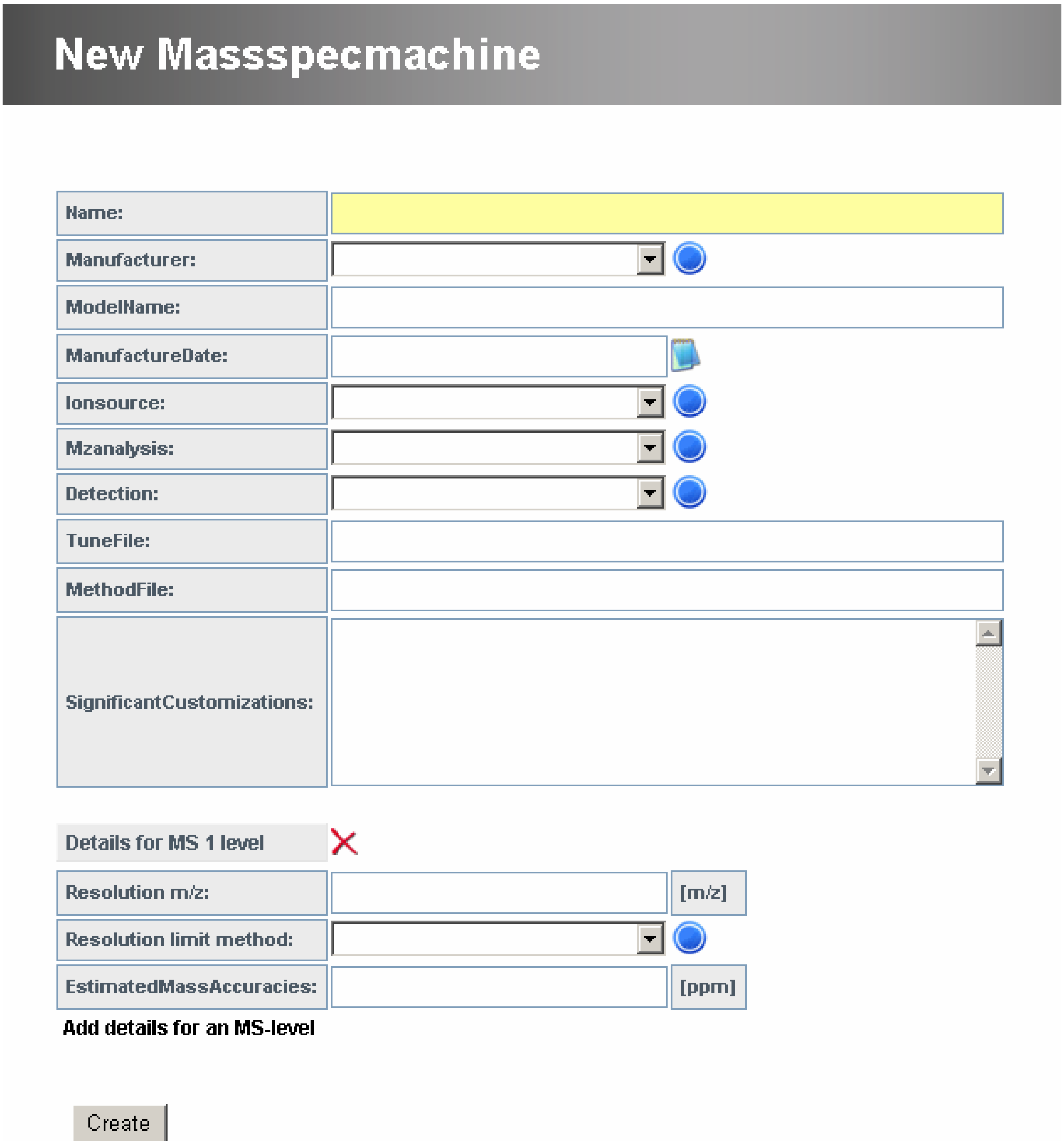
This section is about to describes machine and software settings for the mass spectrometry experiment.

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 only linked to this part. There are two ways how to reach this part. The first one is over 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 Mass Spectrometry->Massspecmachine.



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

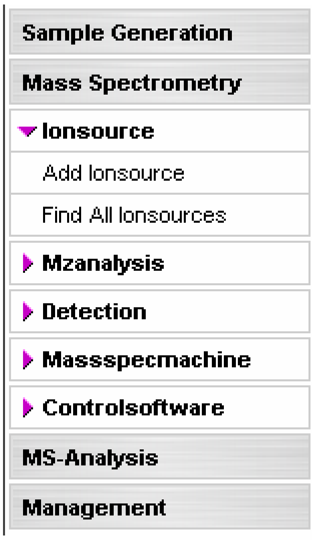


If your desired ionsource,mz analysis or detection is not in the list you can add it directly with the blue button on the right side of the select field. Read more about organisms in chapter 5.2 “Ionsource”, about mz analysis in chapter 5.3 “Mzanalysis” and about detection in chapter 5.4 “Detection”.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

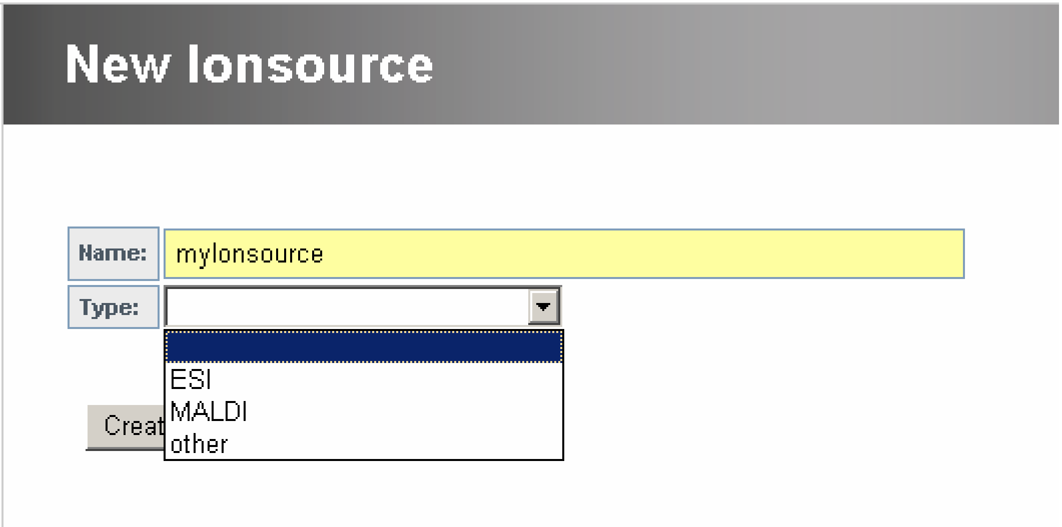
Nr.	Name	ModelName
1	myMassspecmachine	myModel

5.2 Ionsource:

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



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

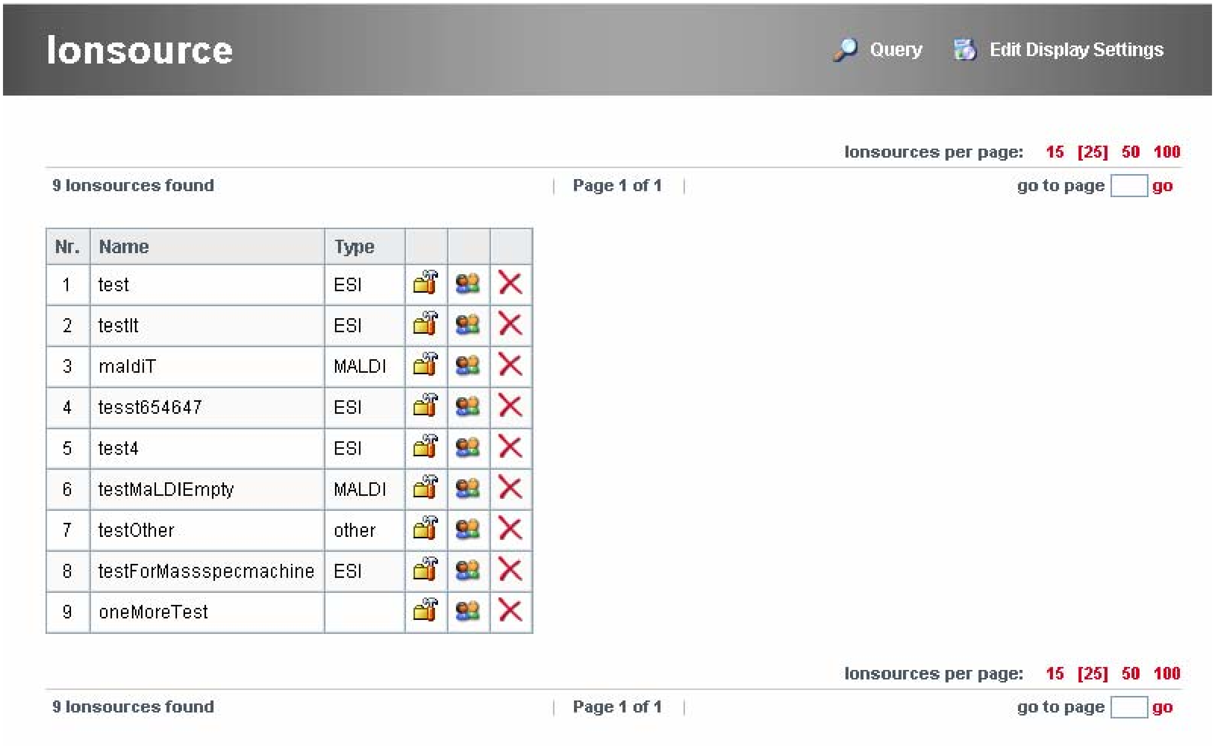


Name: myIonsource

Type:

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:

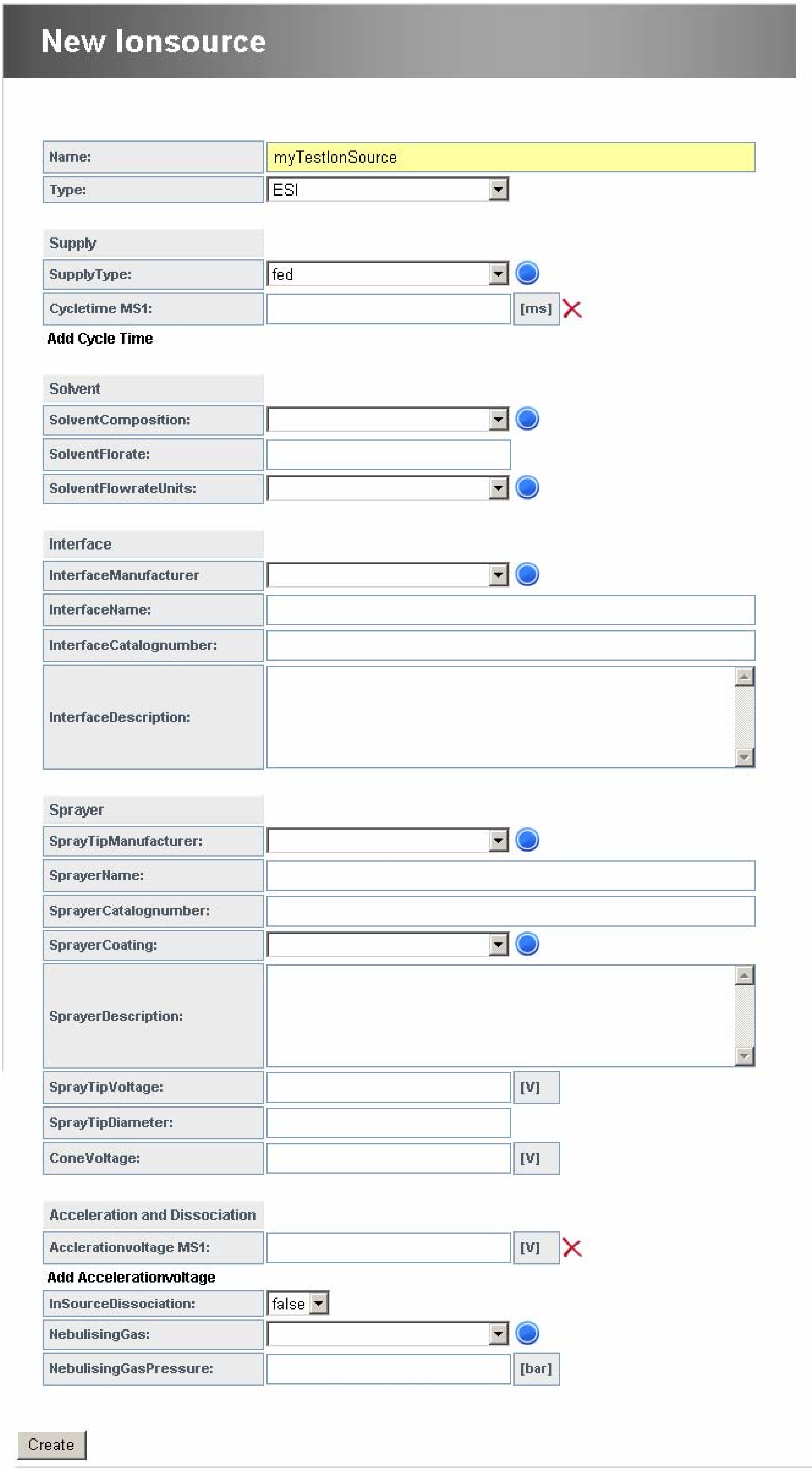


9 Ionsources found | Page 1 of 1 |

Nr.	Name	Type			
1	test	ESI			✕
2	testIt	ESI			✕
3	maldiT	MALDI			✕
4	tesst654647	ESI			✕
5	test4	ESI			✕
6	testMaLDIEmpty	MALDI			✕
7	testOther	other			✕
8	testForMassspecmachine	ESI			✕
9	oneMoreTest				✕

9 Ionsources found | Page 1 of 1 |

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

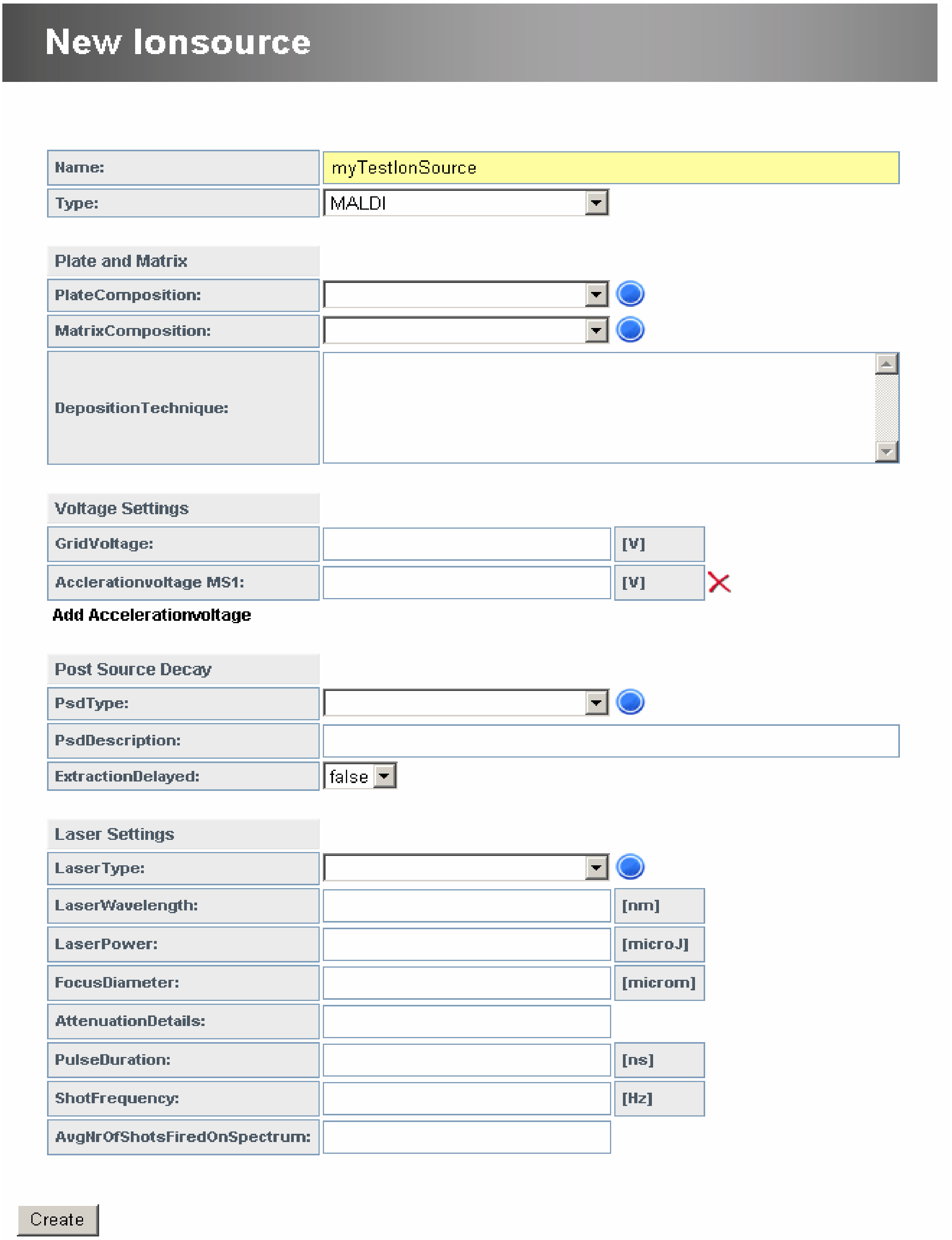
Acclerationvoltage MS1:		[V]

Add Accelerationvoltage

InSourceDissociation:	false	
NebulisingGas:		
NebulisingGasPressure:		[bar]

When you change the type to “ESI” then you get the electro spray input page. 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” exists a second link “Add Accelerationvoltage” where you can enter the acceleration voltages for each MS-level.

5.2.2 MALDI:



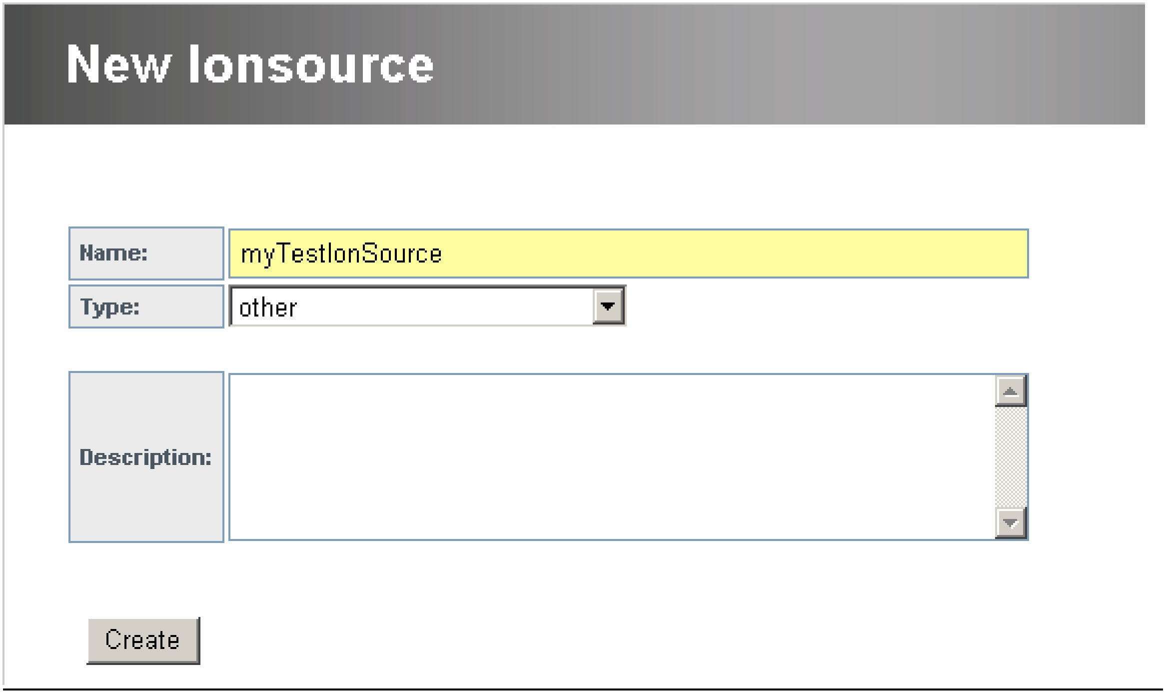
Name: myTestIonSource

Type: MALDI

ExtractionDelayed: false

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

5.2.3 other:

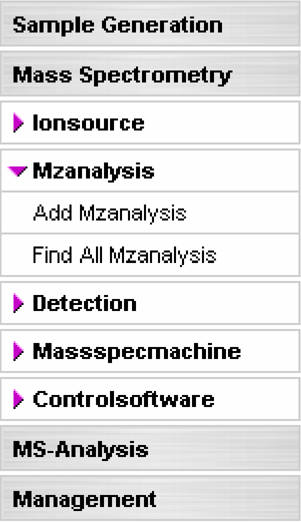


Name: myTestIonSource
Type: other
Description:

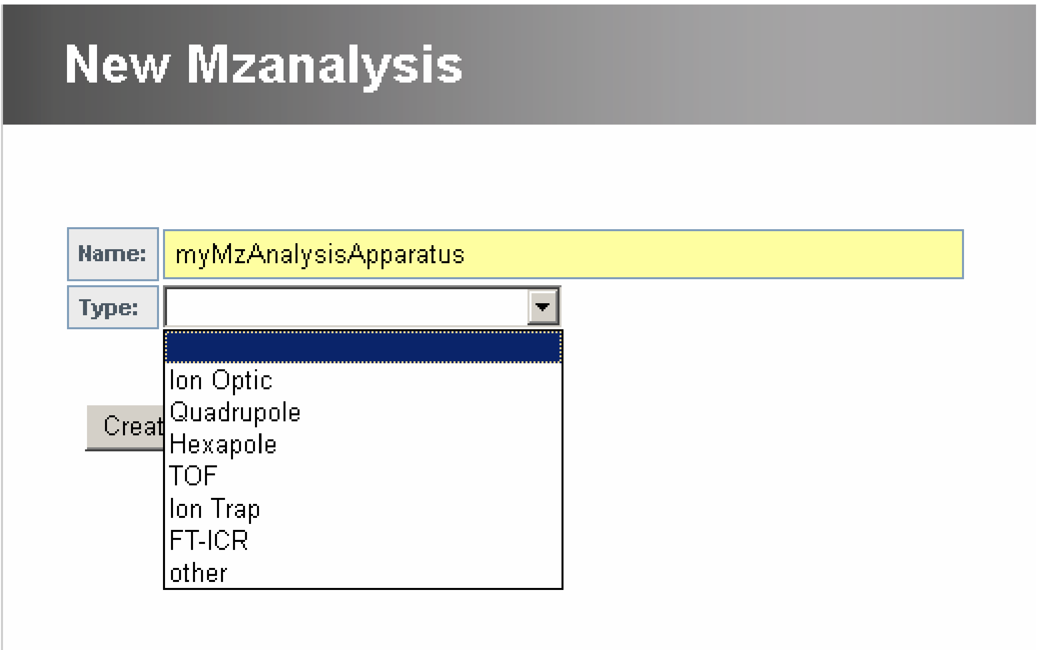
When you change the type to “other” then you get the other ionization input page. There is only an input field for the description of other ionization techniques.

5.3 Mzanalysis:

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



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



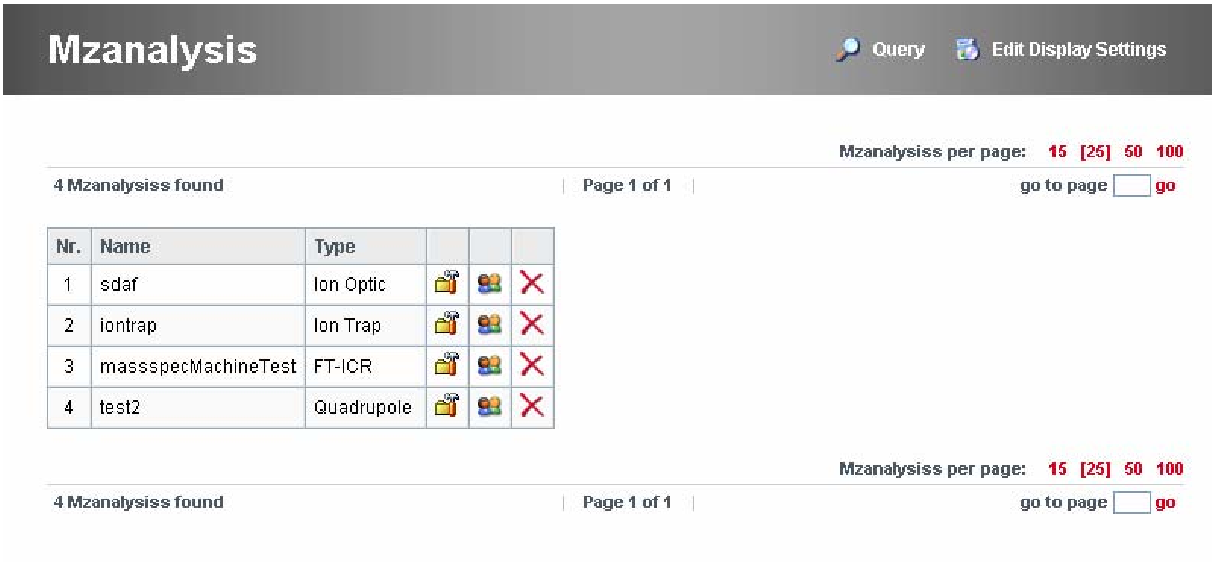
New Mzanalysis

Name: myMzAnalysisApparatus

Type:

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:



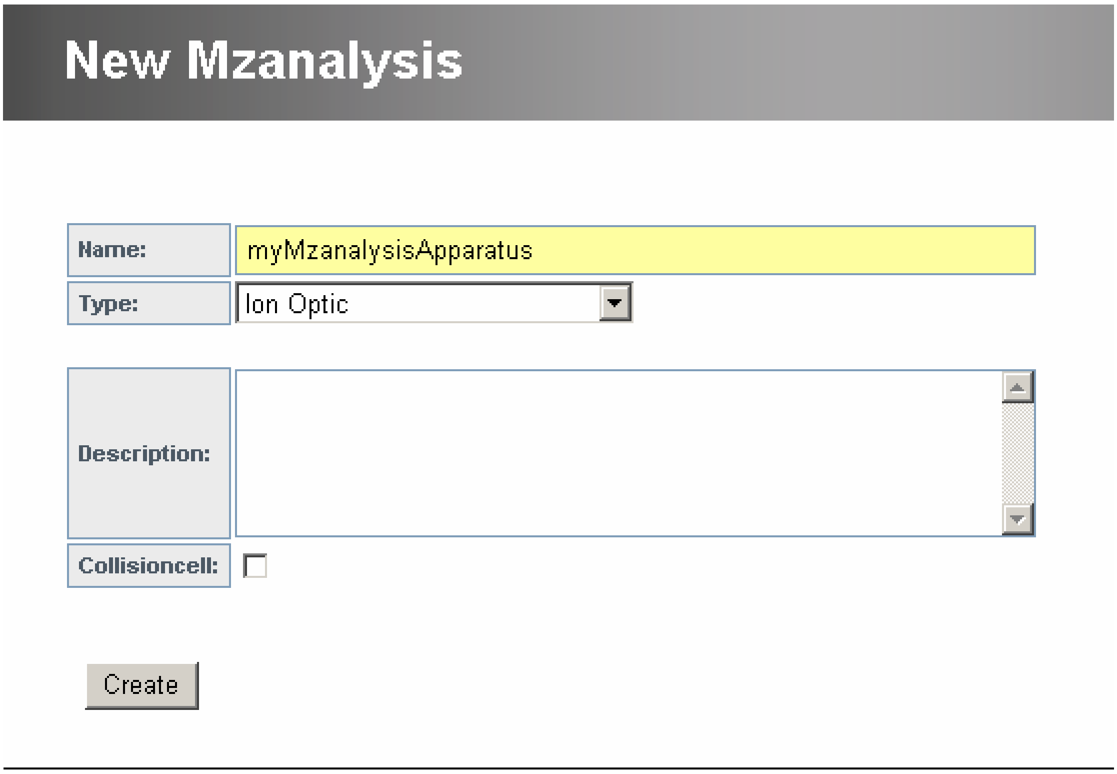
Mzanalysis

4 Mzanalysiss found | Page 1 of 1 |

Nr.	Name	Type			
1	sdaf	Ion Optic			✕
2	iontrap	Ion Trap			✕
3	massspecMachineTest	FT-ICR			✕
4	test2	Quadrupole			✕

4 Mzanalysiss found | Page 1 of 1 |

5.3.1 Ion optic:


New Mzanalysis

Name: myMzanalysisApparatus

Type: Ion Optic

Description:

Collisioncell: ☐

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).

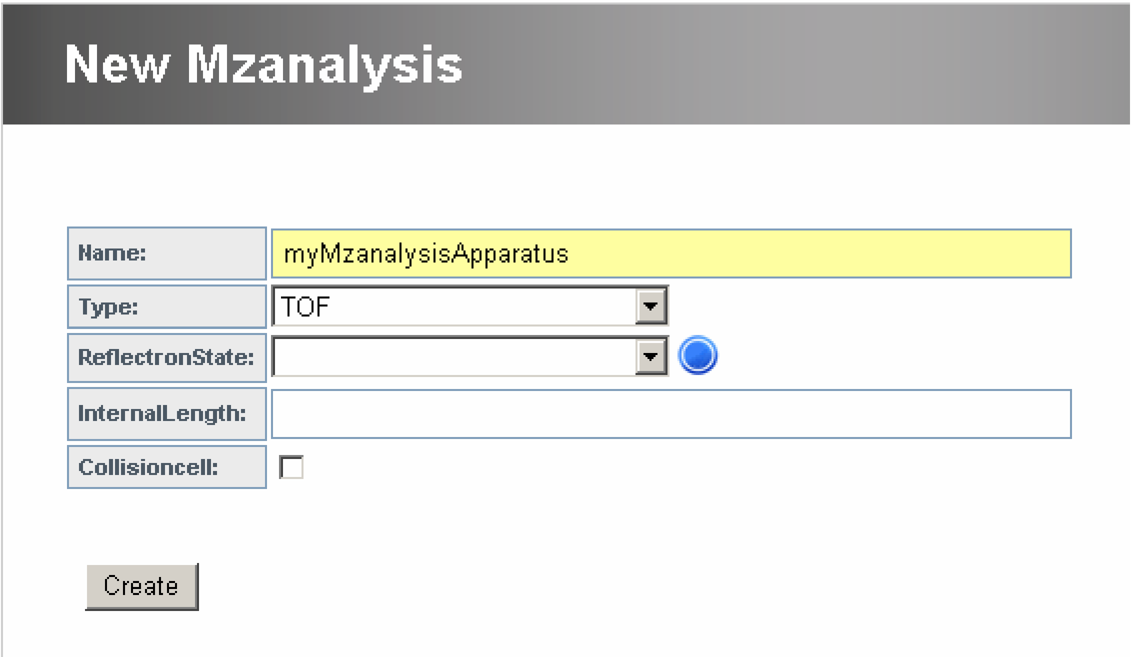
5.3.2 Quadrupole:

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:


New Mzanalysis

Name: myMzanalysisApparatus

Type: TOF

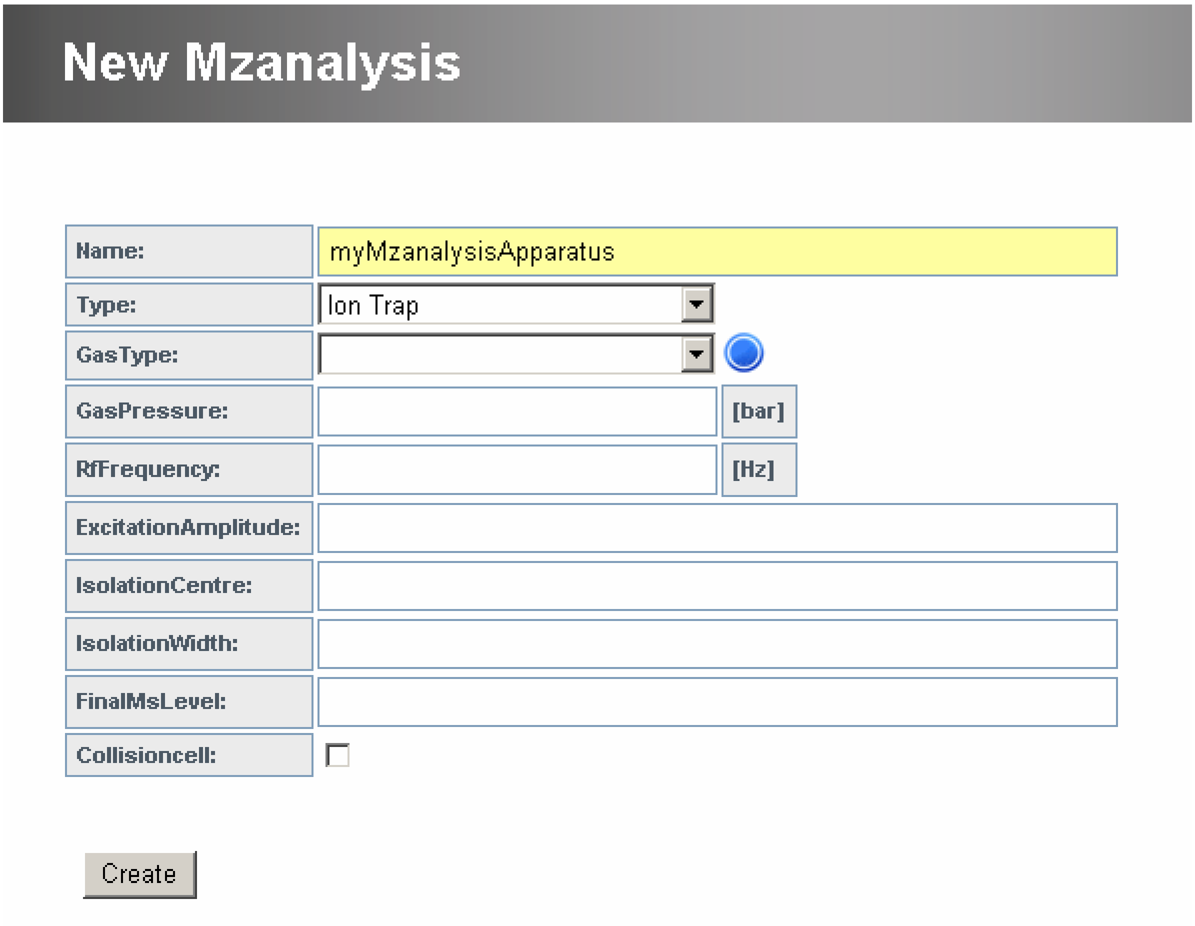
ReflectronState:

InternalLength:

Collisioncell: ☐

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:



New Mzanalysis

Name:	myMzanalysisApparatus
Type:	Ion Trap
GasType:	
GasPressure:	[bar]
RfFrequency:	[Hz]
ExcitationAmplitude:	
IsolationCentre:	
IsolationWidth:	
FinalMsLevel:	
Collisioncell:	☐

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).

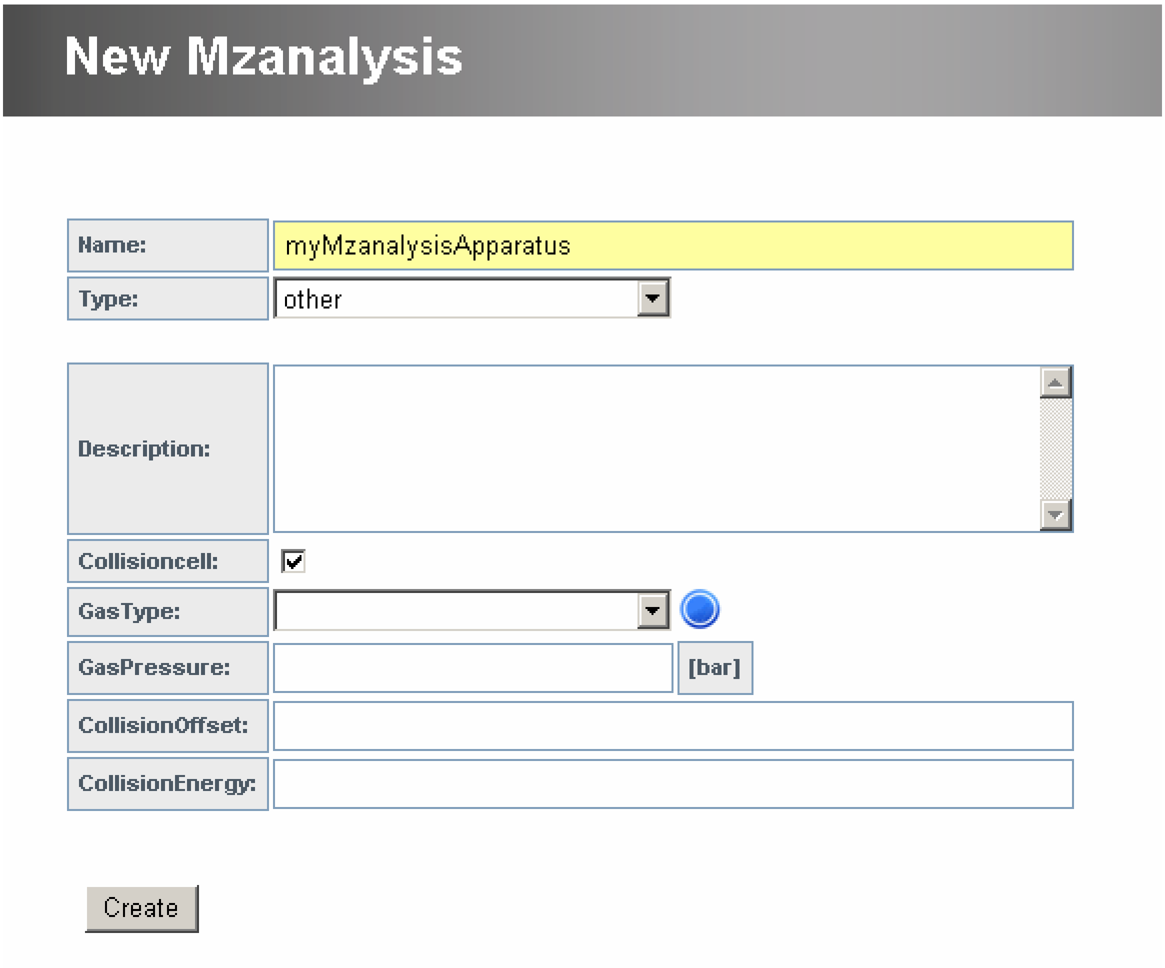
5.3.6 FT-ICR:

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:



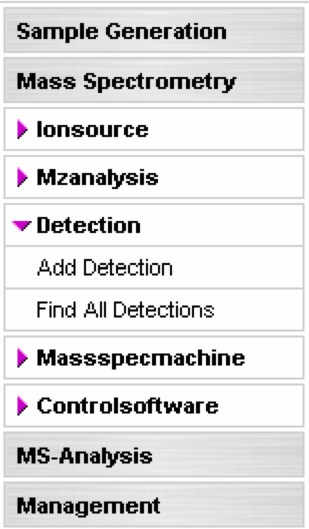
New Mzanalysis

Name:	myMzanalysisApparatus
Type:	other
Description:	
Collisioncell:	☑
GasType:	
GasPressure:	[bar]
CollisionOffset:	
CollisionEnergy:	

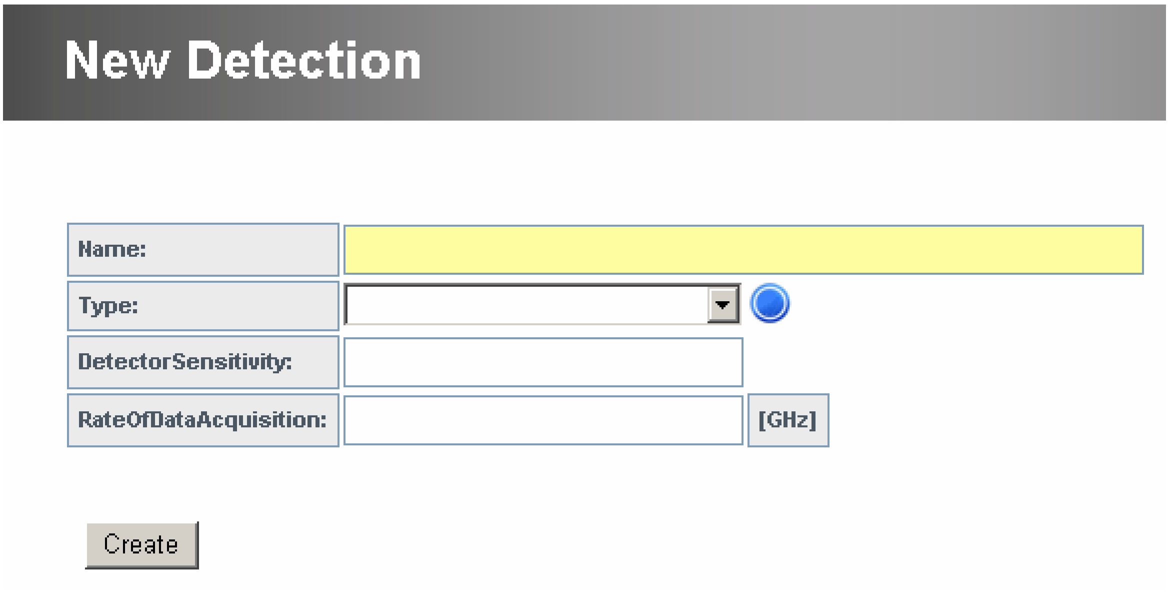
When you check the "Collision cell" check box you can enter information about the collision cell.

5.4 Detection:

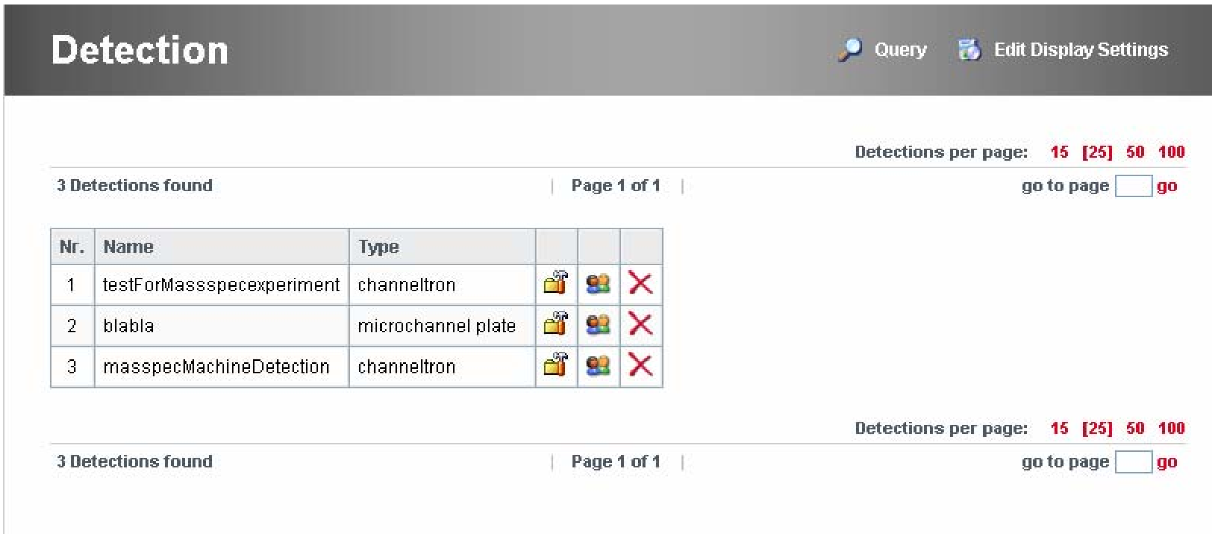
By clicking Mass Spectrometry->Detection you reach the detection section.



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:



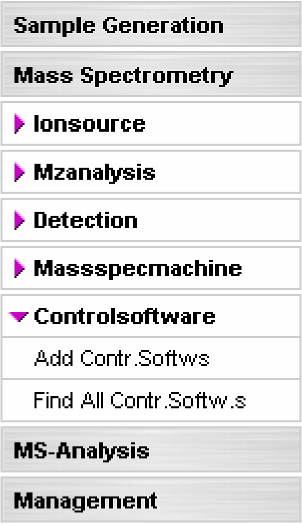
3 Detections found | Page 1 of 1 |

Nr.	Name	Type			
1	testForMassspecexperiment	channeltron			✕
2	blabla	microchannel plate			✕
3	masspecMachineDetection	channeltron			✕

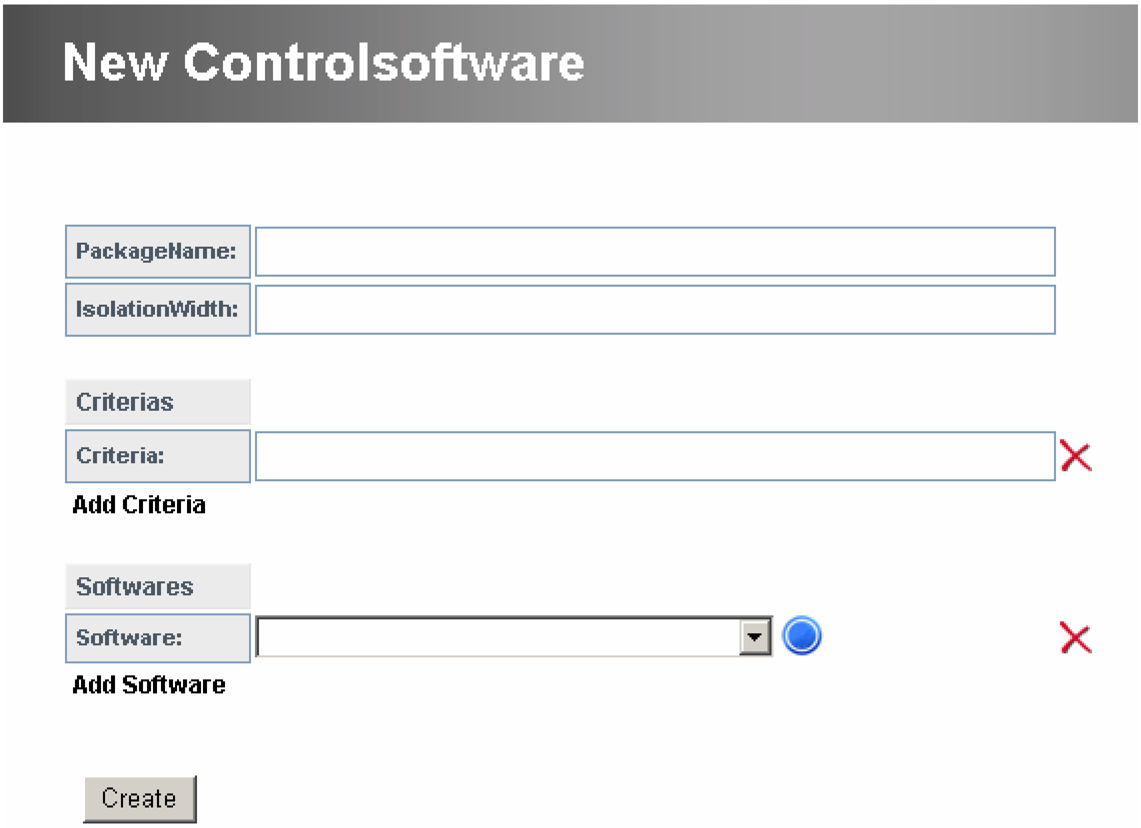
3 Detections found | Page 1 of 1 |

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.

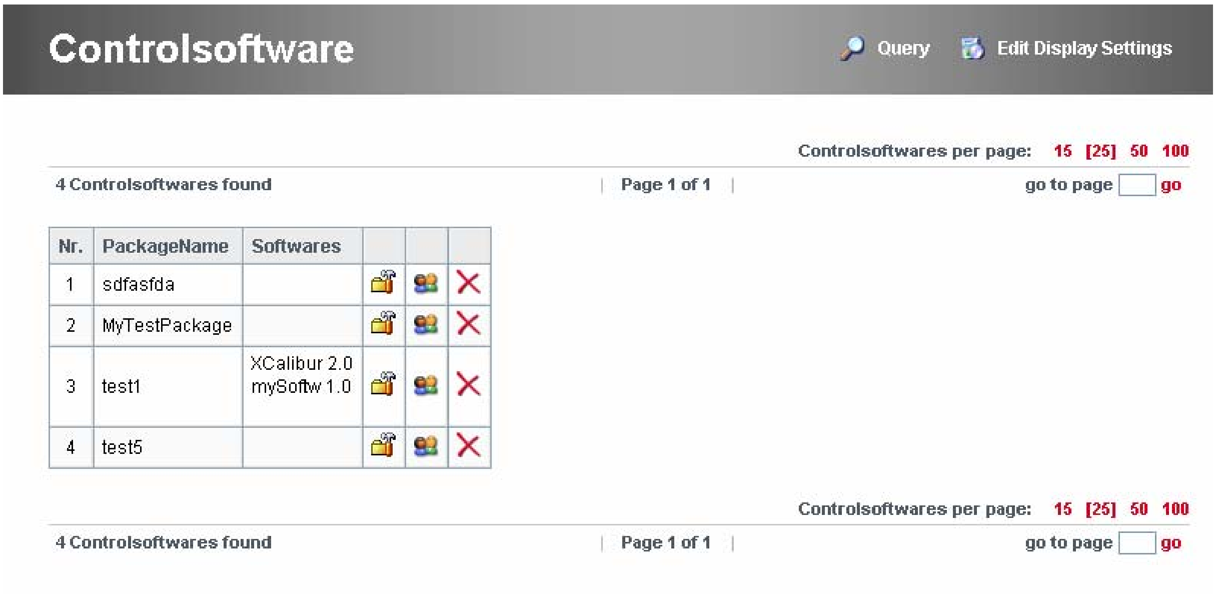


With the “Add Contr.Softws” you can add new control software.



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:



Controlsoftware

Controlsoftwares per page: 15 [25] 50 100

4 Controlsoftwares found | Page 1 of 1 | go to page go

Nr.	PackageName	Softwares			
1	sdfasfda				✕
2	MyTestPackage				✕
3	test1	XCalibur 2.0 mySoftw 1.0			✕
4	test5				✕

Controlsoftwares per page: 15 [25] 50 100

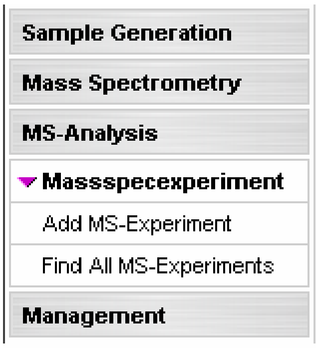
4 Controlsoftwares found | Page 1 of 1 | go to page go

6. Mass Spec Experiment and File Uploading:

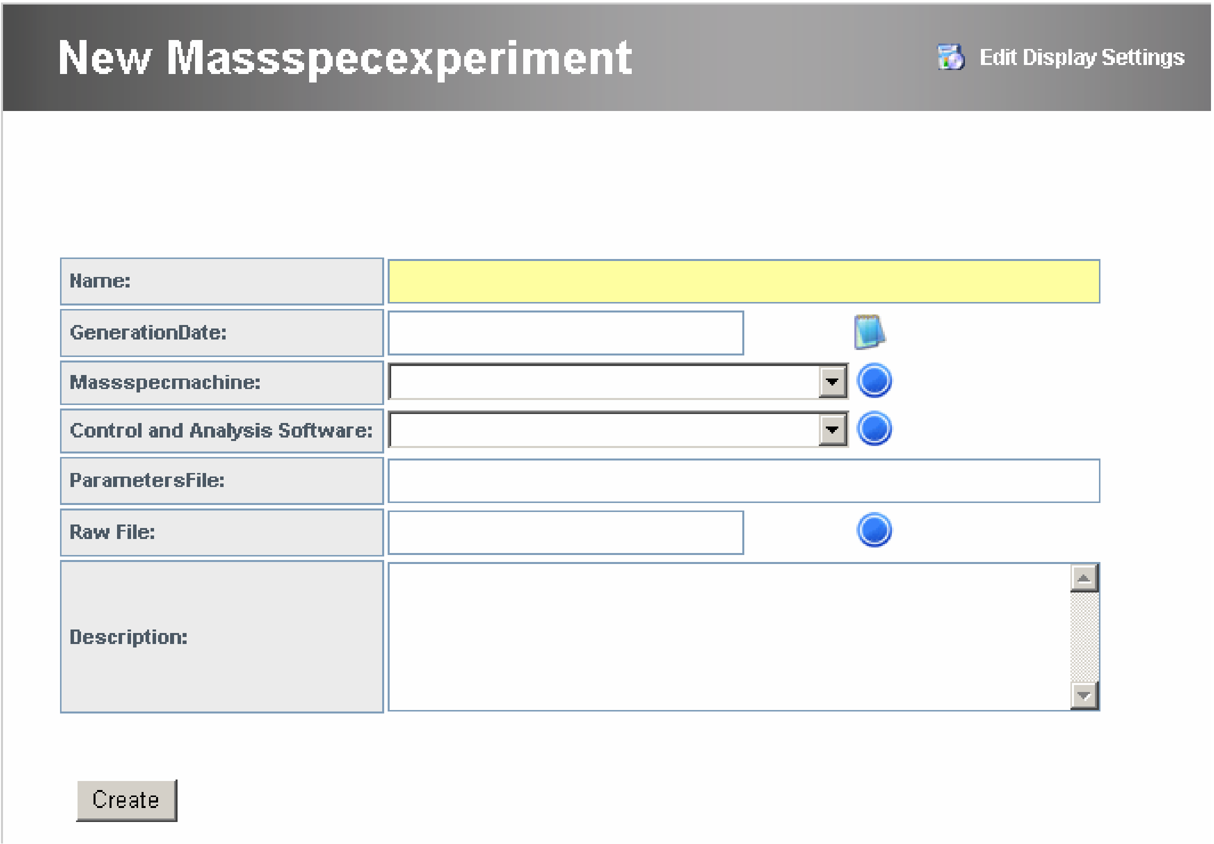
This section describes the generation of mass spectrometry experiments and how you can add searches from different search engines to them.

6.1 Mass spectrometry experiment:

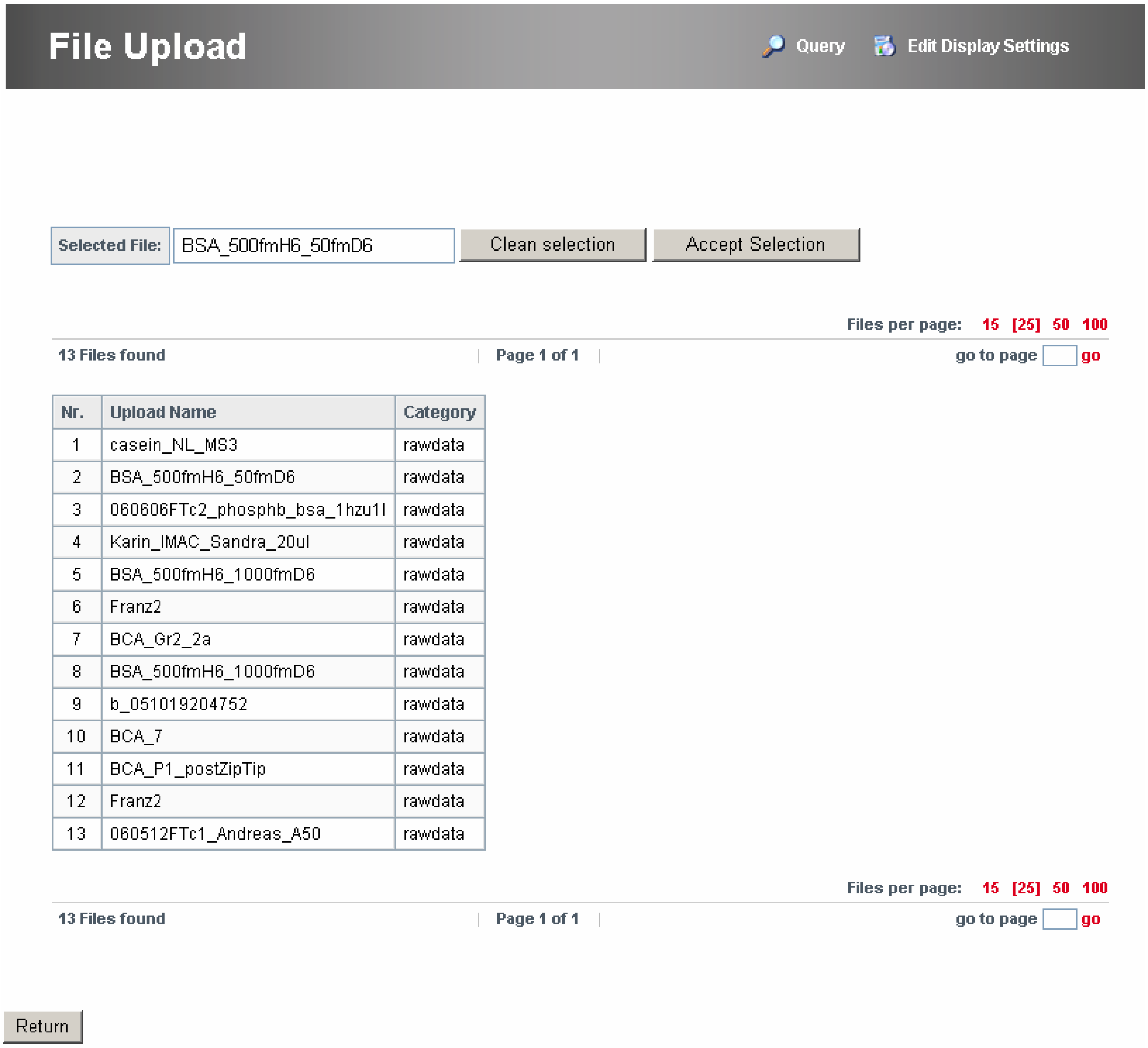
By clicking MS-Analysis->Massspecexperiment you reach the mass spectrometry experiment section. This is a central point, where all the information is linked to one another.



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 you can 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 you to click the blue button next to the “Raw File” input field. The following page will appear:



Selected File: BSA_500fmH6_50fmD6

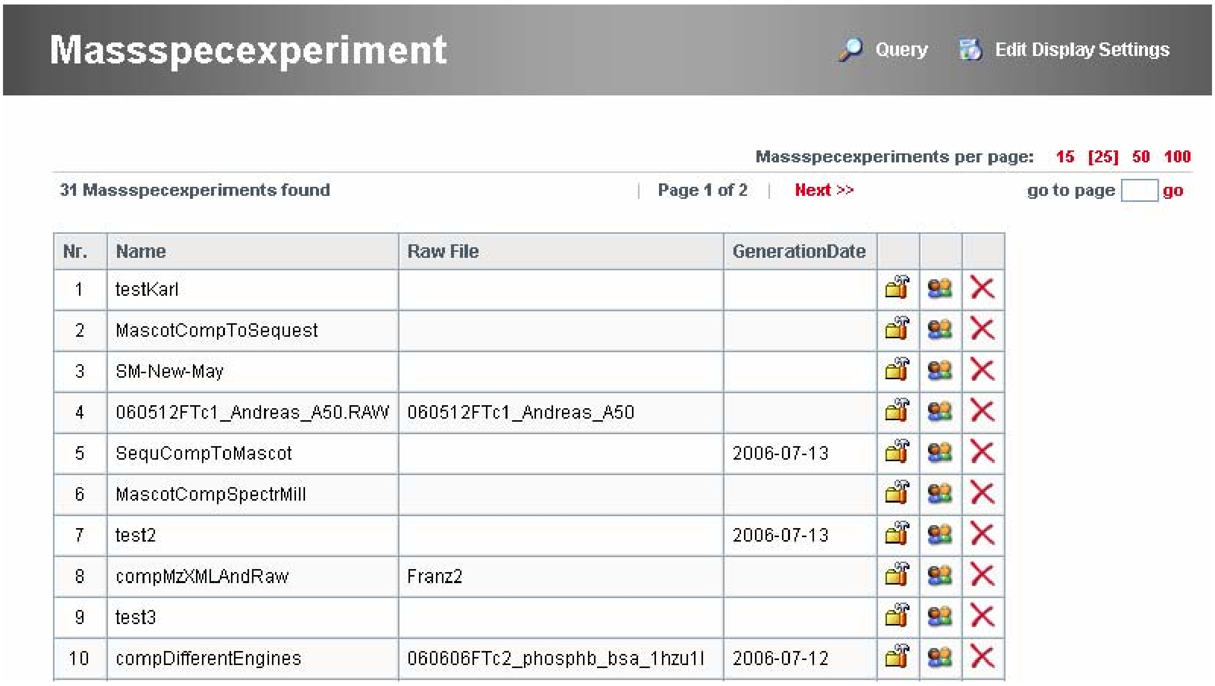
13 Files found | Page 1 of 1 |

Nr.	Upload Name	Category
1	casein_NL_MS3	rawdata
2	BSA_500fmH6_50fmD6	rawdata
3	060606FTc2_phosphb_bsa_1hzu1l	rawdata
4	Karin_IMAC_Sandra_20ul	rawdata
5	BSA_500fmH6_1000fmD6	rawdata
6	Franz2	rawdata
7	BCA_Gr2_2a	rawdata
8	BSA_500fmH6_1000fmD6	rawdata
9	b_051019204752	rawdata
10	BCA_7	rawdata
11	BCA_P1_postZipTip	rawdata
12	Franz2	rawdata
13	060512FTc1_Andreas_A50	rawdata

13 Files found | Page 1 of 1 |

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 mass spectrometry experiment. When 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:

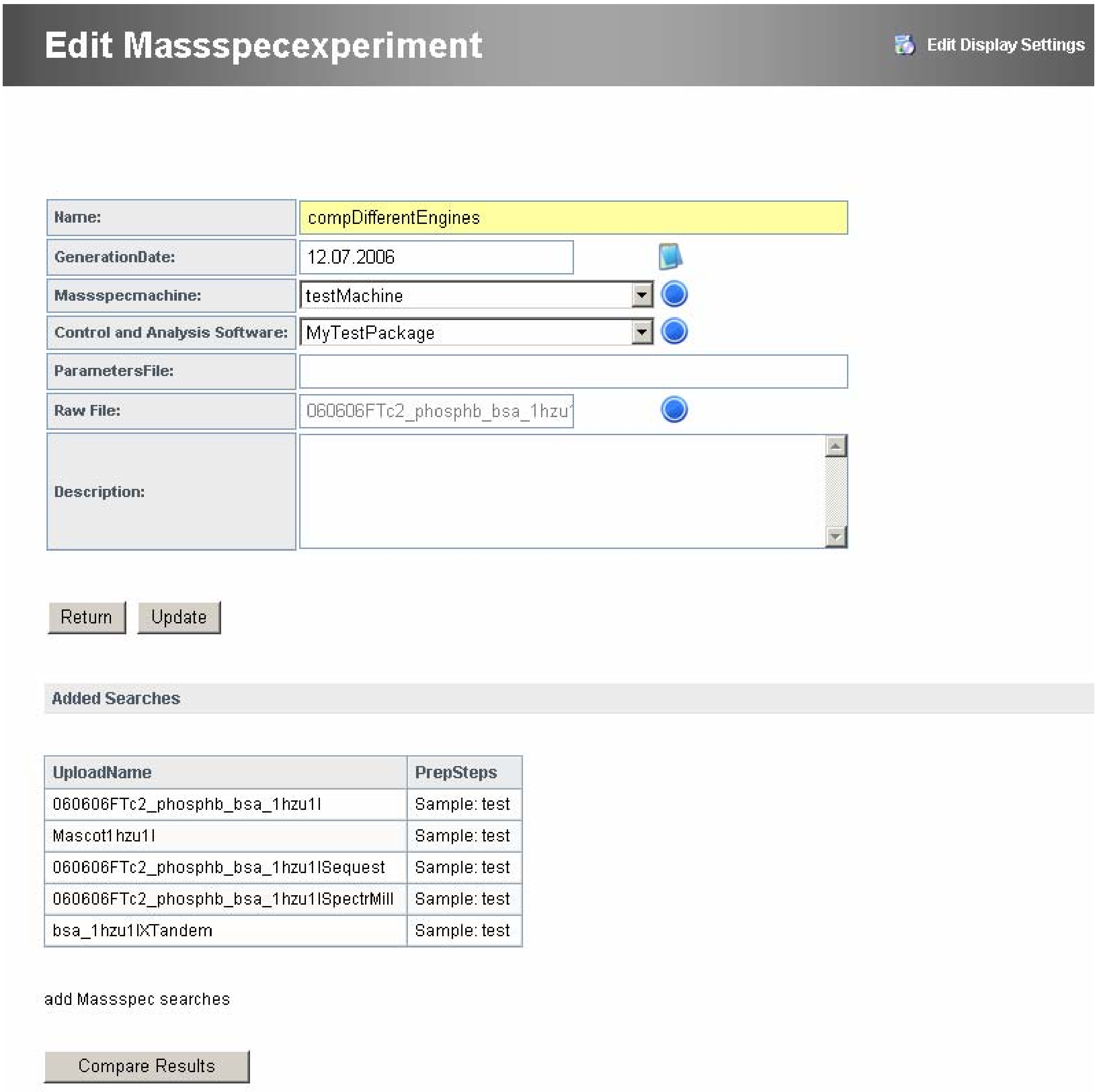


31 Massspecexperiments found

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:



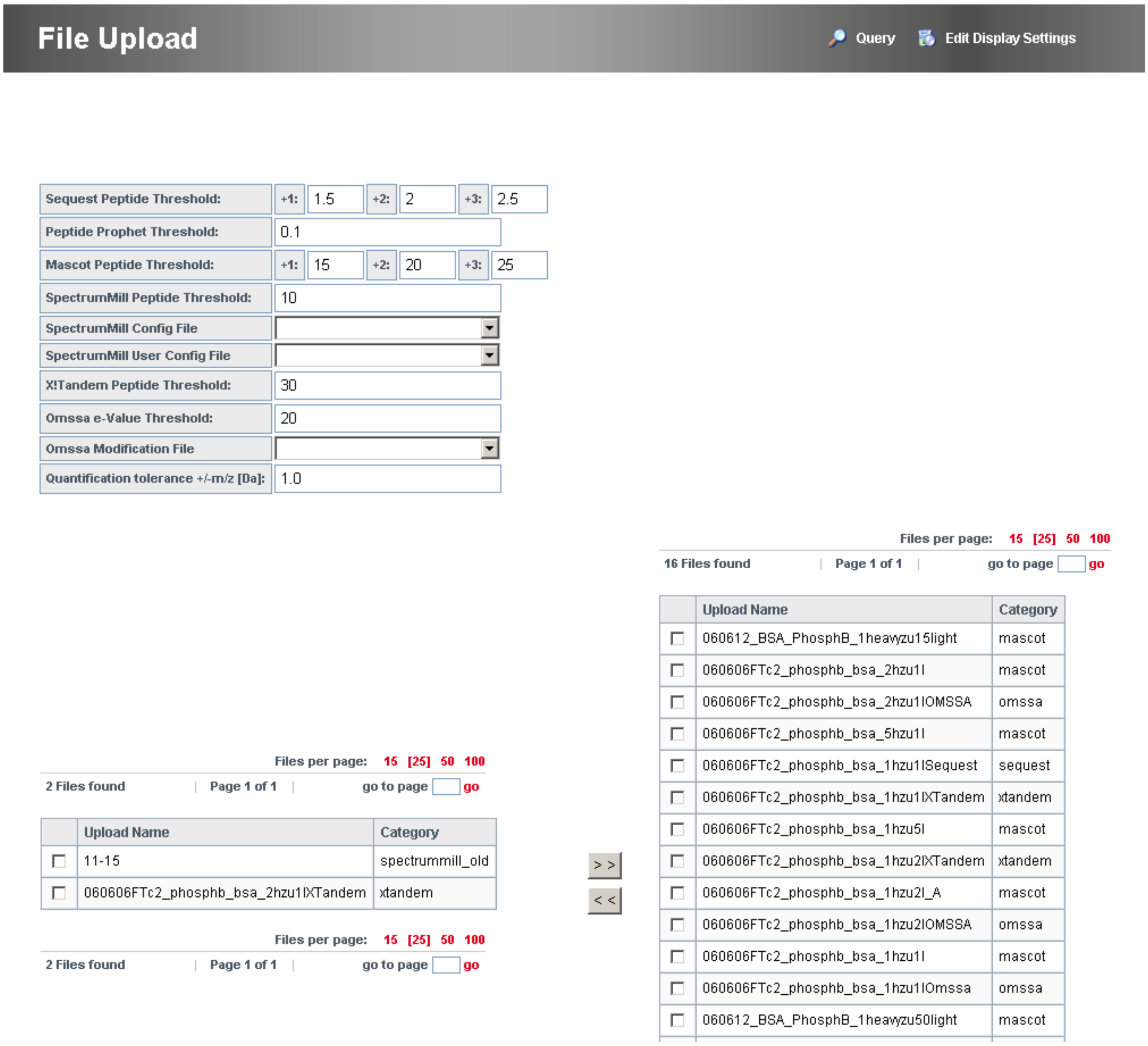
Edit Massspecexperiment

Name:	compDifferentEngines
GenerationDate:	12.07.2006
Massspecmachine:	testMachine
Control and Analysis Software:	MyTestPackage
ParametersFile:	
Raw File:	060606FTc2_phosphb_bsa_1hzu
Description:	

Added Searches

UploadName	PrepSteps
060606FTc2_phosphb_bsa_1hzu1l	Sample: test
Mascot1hzu1l	Sample: test
060606FTc2_phosphb_bsa_1hzu1lSequest	Sample: test
060606FTc2_phosphb_bsa_1hzu1lSpectrMill	Sample: test
bsa_1hzu1lXTandem	Sample: test

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



Sequest Peptide Threshold:	+1: 1.5 +2: 2 +3: 2.5
Peptide Prophet Threshold:	0.1
Mascot Peptide Threshold:	+1: 15 +2: 20 +3: 25
SpectrumMill Peptide Threshold:	10
SpectrumMill Config File	
SpectrumMill User Config File	
X!Tandem Peptide Threshold:	30
Omssa e-Value Threshold:	20
Omssa Modification File	
Quantification tolerance +/-m/z [Da]:	1.0

Files per page: 15 [25] 50 100
2 Files found | Page 1 of 1 | go to page go

	Upload Name	Category
☐	11-15	spectrummill_old
☐	060606FTc2_phosphb_bsa_2hzu1lXTandem	xtandem

Files per page: 15 [25] 50 100
2 Files found | Page 1 of 1 | go to page go

Files per page: 15 [25] 50 100
16 Files found | Page 1 of 1 | go to page go

	Upload Name	Category
☐	060612_BSA_PhosphB_1heavyzu15light	mascot
☐	060606FTc2_phosphb_bsa_2hzu1l	mascot
☐	060606FTc2_phosphb_bsa_2hzu1lOMSSA	omssa
☐	060606FTc2_phosphb_bsa_5hzu1l	mascot
☐	060606FTc2_phosphb_bsa_1hzu1lSequest	sequest
☐	060606FTc2_phosphb_bsa_1hzu1lXTandem	xtandem
☐	060606FTc2_phosphb_bsa_1hzu5l	mascot
☐	060606FTc2_phosphb_bsa_1hzu2lXTandem	xtandem
☐	060606FTc2_phosphb_bsa_1hzu2l_A	mascot
☐	060606FTc2_phosphb_bsa_1hzu2lOMSSA	omssa
☐	060606FTc2_phosphb_bsa_1hzu1l	mascot
☐	060606FTc2_phosphb_bsa_1hzu1lOmssa	omssa
☐	060612_BSA_PhosphB_1heavyzu50light	mascot

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 when you have modificitations added by yourself the Spectrum Mill User Config File (smconfig.custom.xml). For OMSSA you have to specify the Omssa Modifications File (mods.xml).

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

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:

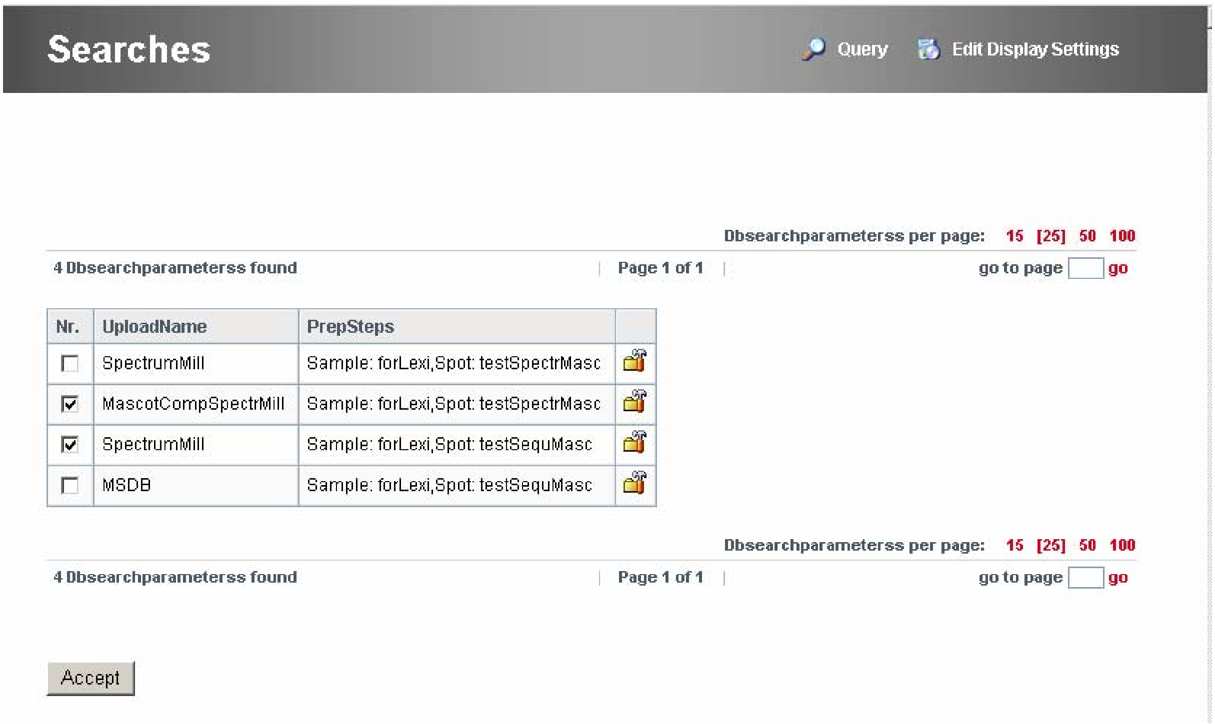
1. To click directly on the upload name table below the mass spectrometry experiment (see first picture section 6.2 "File parsing into MASPECTRAS")
2. To use the

   Compare Results

   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 out of the uploaded searches which ones you want to compare. All of the uploaded searches below this data point are displayed. The preparation steps that have been used are visible there as well.



Dbsearchparameterss per page: 15 [25] 50 100

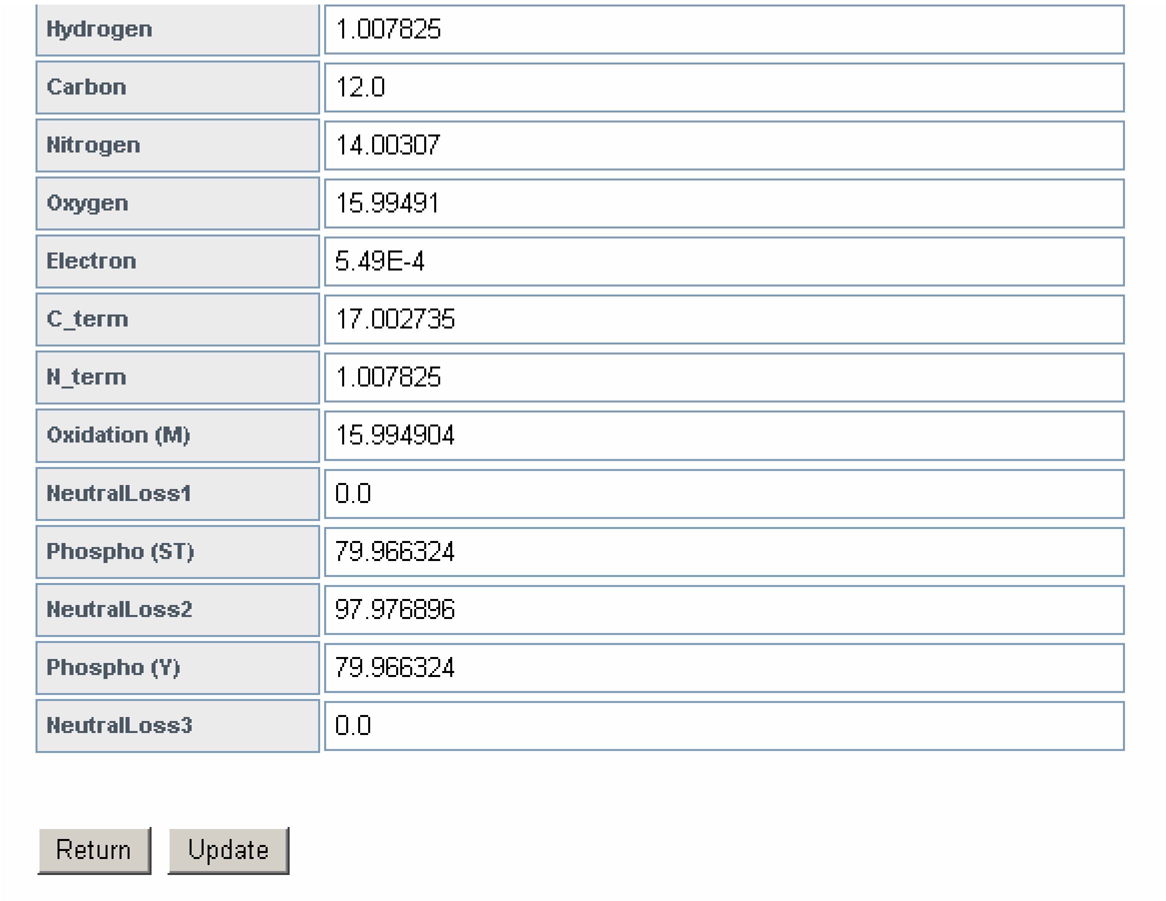
4 Dbsearchparameterss found | Page 1 of 1 | go to page go

Nr.	UploadName	PrepSteps	
☐	SpectrumMill	Sample: forLexi,Spot: testSpectrMasc	
☑	MascotCompSpectrMill	Sample: forLexi,Spot: testSpectrMasc	
☑	SpectrumMill	Sample: forLexi,Spot: testSequMasc	
☐	MSDB	Sample: forLexi,Spot: testSequMasc	

Dbsearchparameterss per page: 15 [25] 50 100

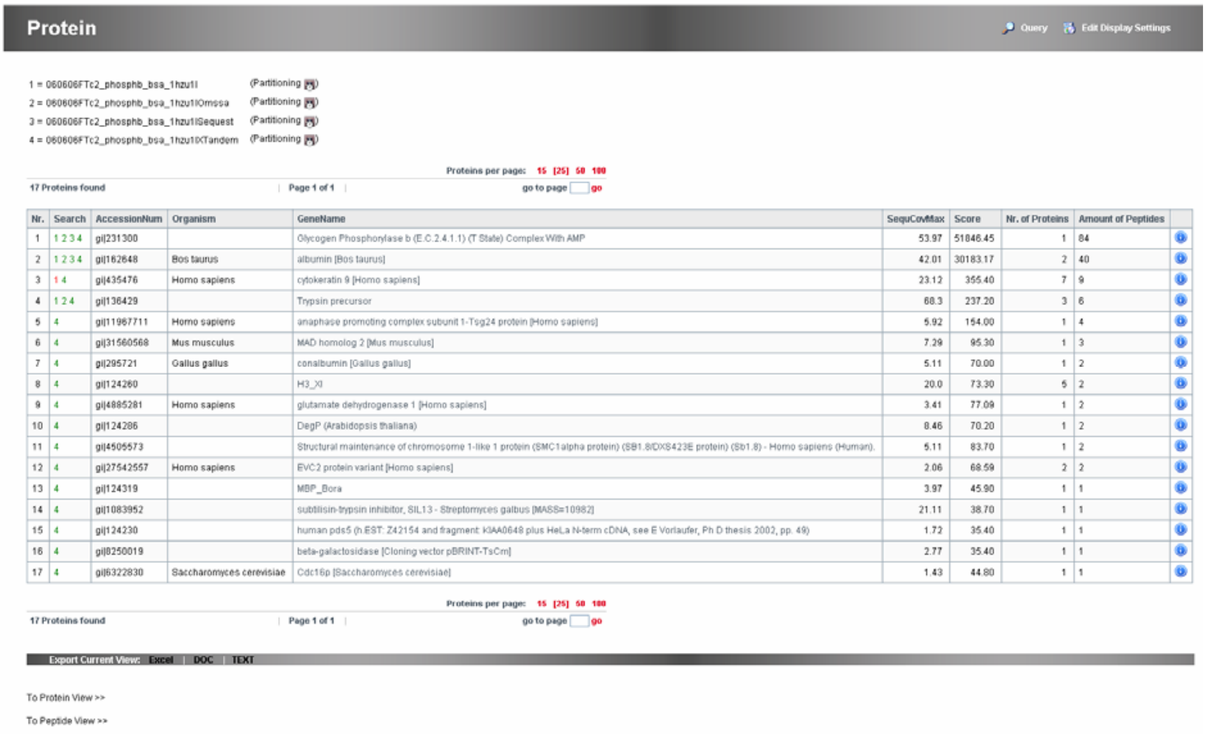
4 Dbsearchparameterss found | Page 1 of 1 | go to page go

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

7.1 Protein comparison:



1 = 060606FTc2_phosphb_bsa_1hzu1I (Partitioning)
2 = 060606FTc2_phosphb_bsa_1hzu1IOmssa (Partitioning)
3 = 060606FTc2_phosphb_bsa_1hzu1ISequest (Partitioning)
4 = 060606FTc2_phosphb_bsa_1hzu1IXTandem (Partitioning)

Proteins per page: 15 [25] 50 100

17 Proteins found | Page 1 of 1 | go to page go

Nr.	Search	AccessionNum	Organism	GeneName	SequCovMax	Score	Nr. of Proteins	Amount of Peptides	
1	1 2 3 4	gi|231300		Glycogen Phosphorylase b (E.C.2.4.1.1) (T State) Complex With AMP	53.97	51846.45	1	84	ⓘ
2	1 2 3 4	gi|162648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	2	40	ⓘ
3	1 4	gi|435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	355.40	7	9	ⓘ
4	1 2 4	gi|136429		Trypsin precursor	68.3	237.20	3	6	ⓘ
5	4	gi|11967711	Homo sapiens	anaphase promoting complex subunit 1-Tsg24 protein [Homo sapiens]	5.92	154.00	1	4	ⓘ
6	4	gi|31560568	Mus musculus	MAD homolog 2 [Mus musculus]	7.29	95.30	1	3	ⓘ
7	4	gi|295721	Gallus gallus	conalbumin [Gallus gallus]	5.11	70.00	1	2	ⓘ
8	4	gi|124260		H3_XI	20.0	73.30	5	2	ⓘ
9	4	gi|4885281	Homo sapiens	glutamate dehydrogenase 1 [Homo sapiens]	3.41	77.09	1	2	ⓘ
10	4	gi|124286		DegP (Arabidopsis thaliana)	8.46	70.20	1	2	ⓘ
11	4	gi|4505573		Structural maintenance of chromosome 1-like 1 protein (SMC1alpha protein) (SB1.8/DXS423E protein) (Sb1.8) - Homo sapiens (Human).	5.11	83.70	1	2	ⓘ
12	4	gi|27542557	Homo sapiens	EVC2 protein variant [Homo sapiens]	2.06	68.59	2	2	ⓘ
13	4	gi|124319		MBP_Bora	3.97	45.90	1	1	ⓘ
14	4	gi|1083952		subtilisin-trypsin inhibitor, SIL13 - Streptomyces galbus [MASS=10982]	21.11	38.70	1	1	ⓘ
15	4	gi|124230		human pds5 (h.EST: Z42154 and fragment: KIAA0648 plus HeLa N-term cDNA, see E Vorlaufer, Ph D thesis 2002, pp. 49)	1.72	35.40	1	1	ⓘ
16	4	gi|8250019		beta-galactosidase [Cloning vector pBRINT-TsCm]	2.77	35.40	1	1	ⓘ
17	4	gi|6322830	Saccharomyces cerevisiae	Cdc16p [Saccharomyces cerevisiae]	1.43	44.80	1	1	ⓘ

Proteins per page: 15 [25] 50 100

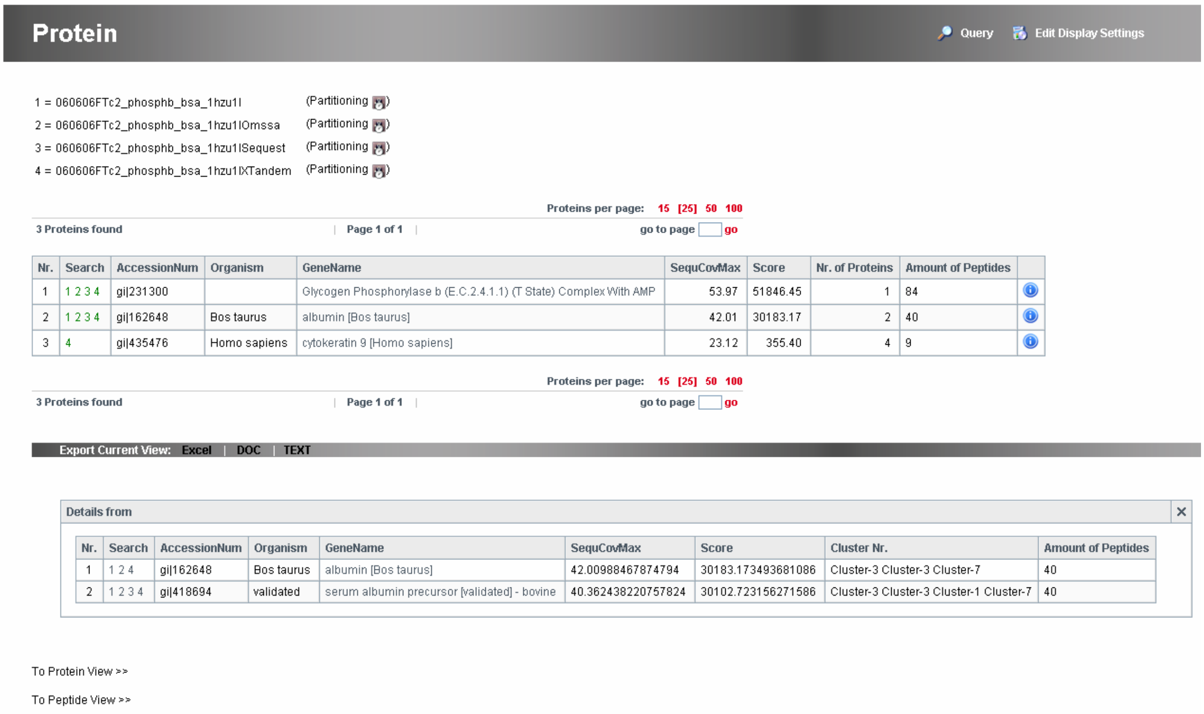
17 Proteins found | Page 1 of 1 | go to page go

Export Current View: Excel | DOC | TEXT

To Protein View >>

To Peptide View >>

Below the header the searches that you have selected are listed by name and a number is assigned to find it in the table below. Next to the names there is a link in brackets called "Partitioning". With this link you reach a page with a closer description of the cluster (7.2). In the table below the found proteins are listed. 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 number indicates the search where the protein has been found in. 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.



1 = 060606FTc2_phosphb_bsa_1hzu1I (Partitioning)
2 = 060606FTc2_phosphb_bsa_1hzu1IOmssa (Partitioning)
3 = 060606FTc2_phosphb_bsa_1hzu1ISequest (Partitioning)
4 = 060606FTc2_phosphb_bsa_1hzu1IXTandem (Partitioning)

Proteins per page: 15 [25] 50 100
3 Proteins found | Page 1 of 1 | go to page go

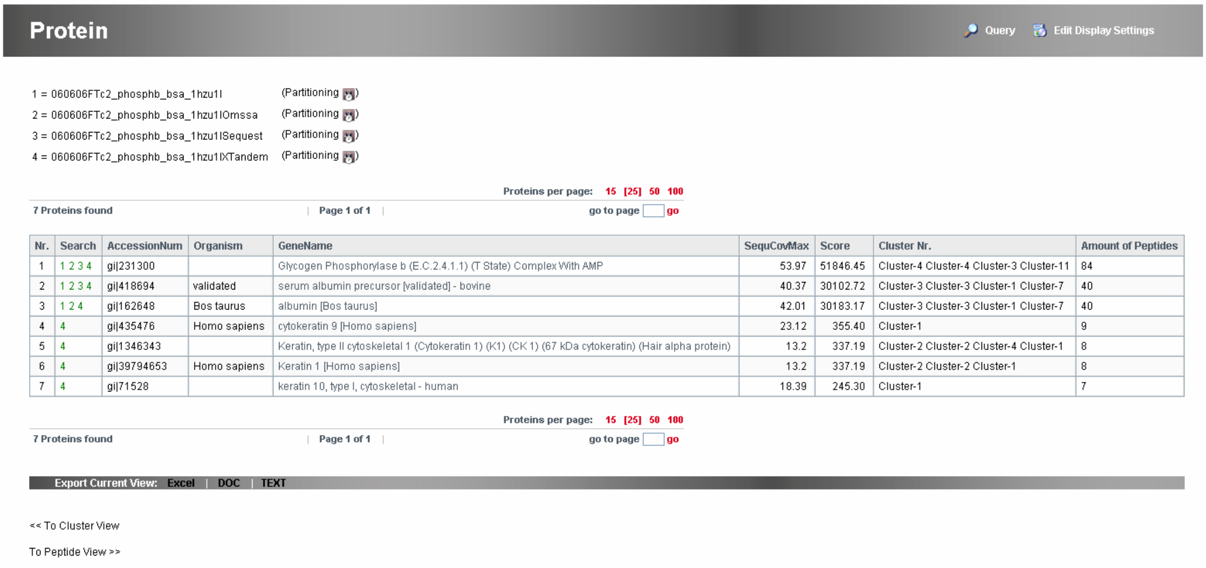
Nr.	Search	AccessionNum	Organism	GeneName	SequCovMax	Score	Nr. of Proteins	Amount of Peptides	
1	1 2 3 4	gi|231300		Glycogen Phosphorylase b (E.C.2.4.1.1) (T State) Complex With AMP	53.97	51846.45	1	84	ⓘ
2	1 2 3 4	gi|162648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	2	40	ⓘ
3	4	gi|435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	355.40	4	9	ⓘ

Proteins per page: 15 [25] 50 100
3 Proteins found | Page 1 of 1 | go to page go

Details from

Nr.	Search	AccessionNum	Organism	GeneName	SequCovMax	Score	Cluster Nr.	Amount of Peptides
1	1 2 4	gi|162648	Bos taurus	albumin [Bos taurus]	42.00988467874794	30183.173493681086	Cluster-3 Cluster-3 Cluster-7	40
2	1 2 3 4	gi|418694	validated	serum albumin precursor [validated] - bovine	40.362438220757824	30102.723156271586	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40

The “Cluster Nr.” indicates the cluster where the protein is located. The order is the same like the numbers in the “Search” column are ordered.
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 and you will get all proteins displayed.



1 = 060606FTc2_phosphb_bsa_1hzu1I (Partitioning)
2 = 060606FTc2_phosphb_bsa_1hzu1IOmssa (Partitioning)
3 = 060606FTc2_phosphb_bsa_1hzu1ISequest (Partitioning)
4 = 060606FTc2_phosphb_bsa_1hzu1IXTandem (Partitioning)

Proteins per page: 15 [25] 50 100
7 Proteins found | Page 1 of 1 | go to page go

Nr.	Search	AccessionNum	Organism	GeneName	SequCovMax	Score	Cluster Nr.	Amount of Peptides
1	1 2 3 4	gi|231300		Glycogen Phosphorylase b (E.C.2.4.1.1) (T State) Complex With AMP	53.97	51846.45	Cluster-4 Cluster-4 Cluster-3 Cluster-11	84
2	1 2 3 4	gi|418694	validated	serum albumin precursor [validated] - bovine	40.37	30102.72	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
3	1 2 4	gi|162648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
4	4	gi|435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	355.40	Cluster-1	9
5	4	gi|1346343		Keratin, type II cytoskeletal 1 (Cytokeratin 1) (K1) (CK 1) (67 kDa cytokeratin) (Hair alpha protein)	13.2	337.19	Cluster-2 Cluster-2 Cluster-4 Cluster-1	8
6	4	gi|39794653	Homo sapiens	Keratin 1 [Homo sapiens]	13.2	337.19	Cluster-2 Cluster-2 Cluster-1	8
7	4	gi|71528		keratin 10, type I, cytoskeletal - human	18.39	245.30	Cluster-1	7

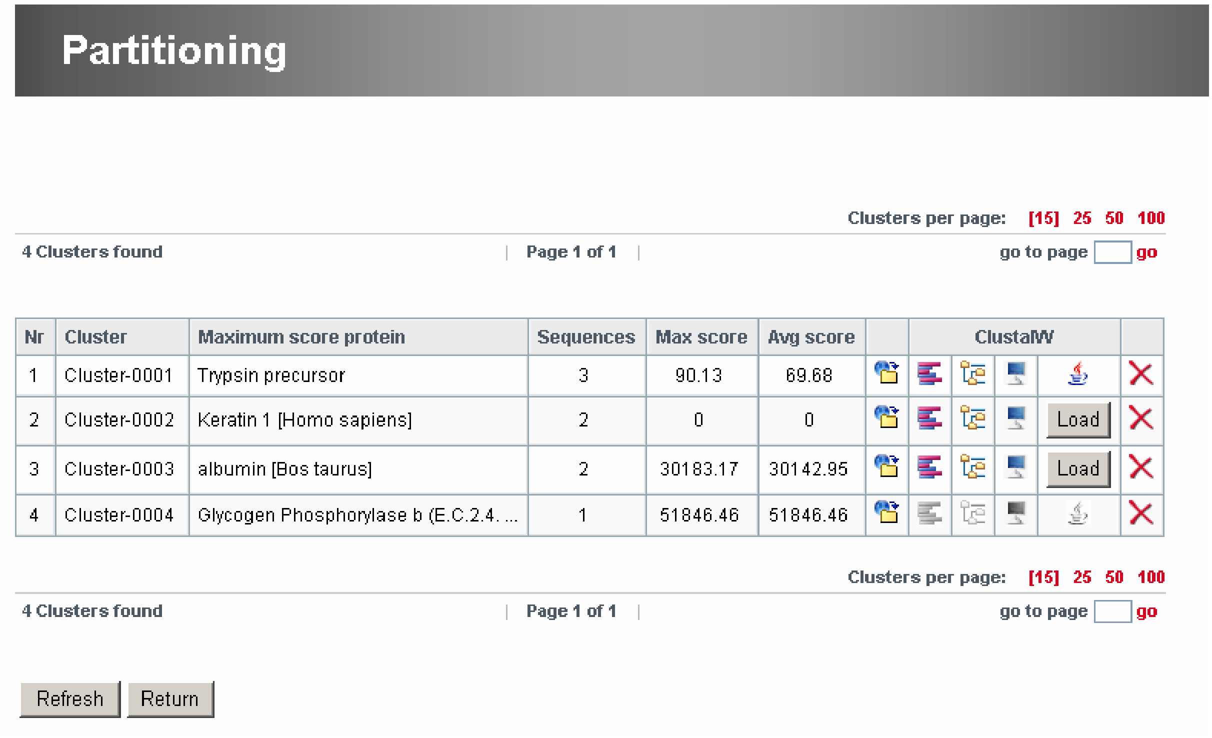
Proteins per page: 15 [25] 50 100
7 Proteins found | Page 1 of 1 | go to page go

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 “>> 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):



Nr	Cluster	Maximum score protein	Sequences	Max score	Avg score		ClustalW				
1	Cluster-0001	Trypsin precursor	3	90.13	69.68					☕	✕
2	Cluster-0002	Keratin 1 [Homo sapiens]	2	0	0					Load	✕
3	Cluster-0003	albumin [Bos taurus]	2	30183.17	30142.95					Load	✕
4	Cluster-0004	Glycogen Phosphorylase b (E.C.2.4. ...	1	51846.46	51846.46					☕	✕

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

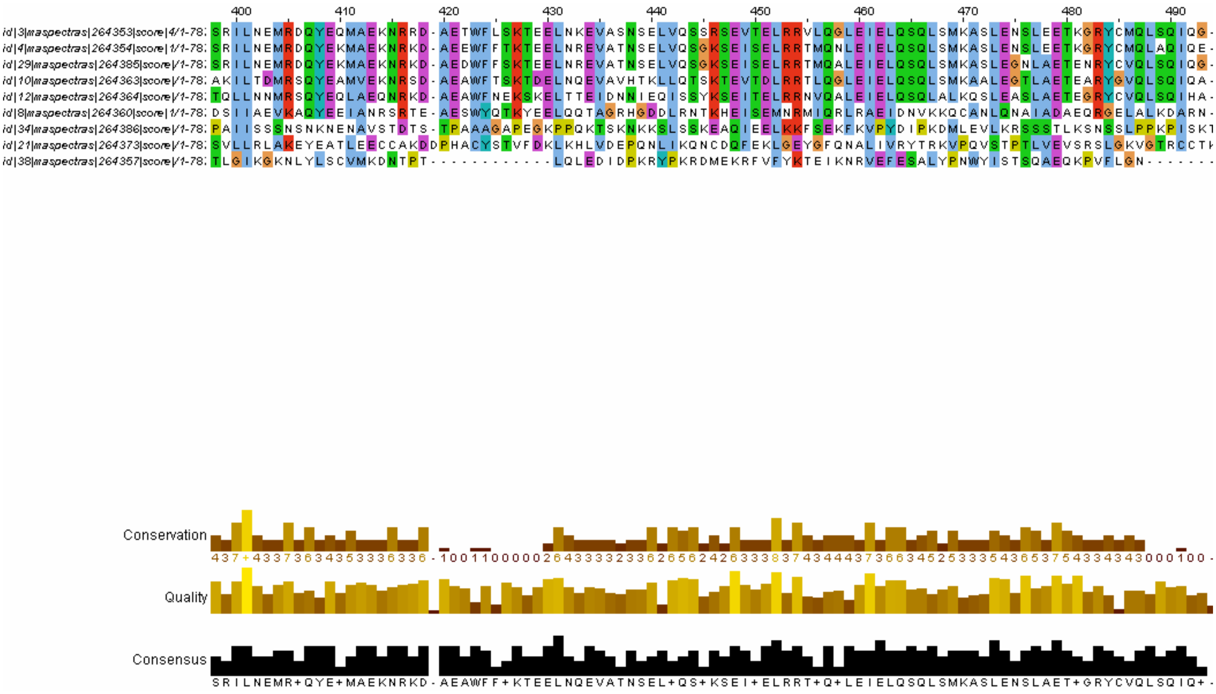
: Download of the alignment of the proteins

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

: The log-file of the alignment

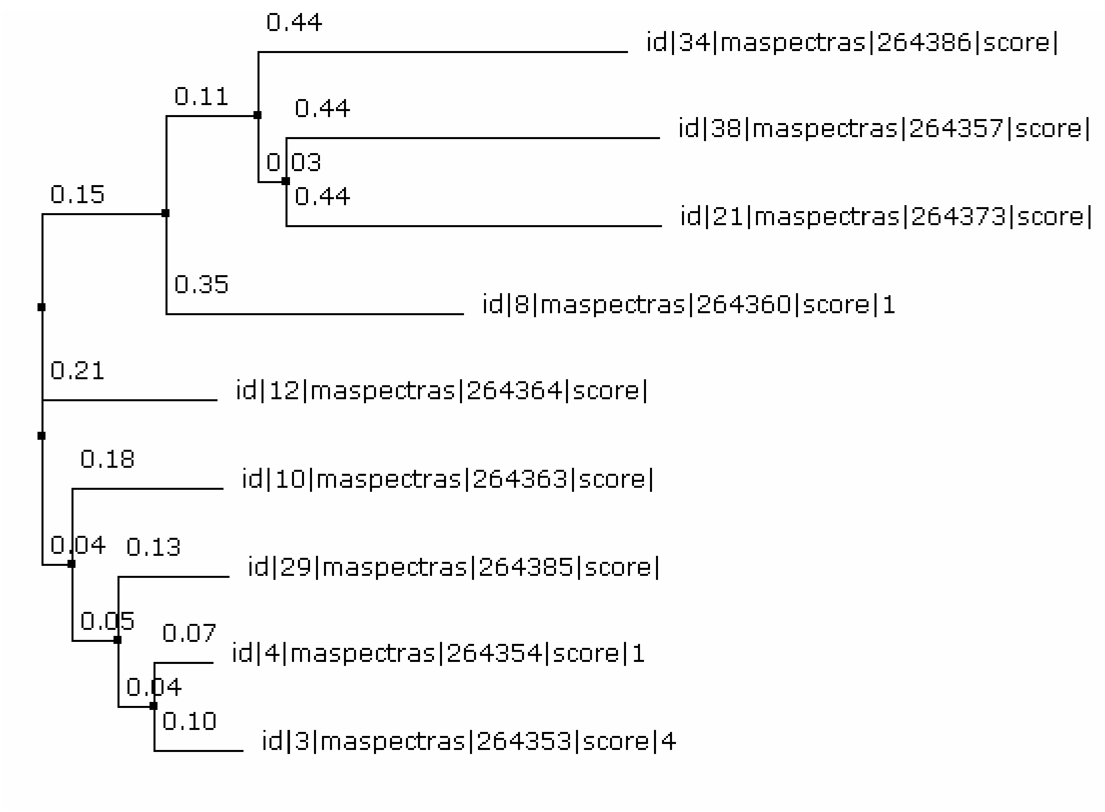
Load : The ☕ is a applet itself and when you want to display a big list all of the applets would have to be loaded and takes to much time. Therefore the “Load” button has to be presses to get the corresponding applet.

☕ : Starts Jalview applet to see the alignment

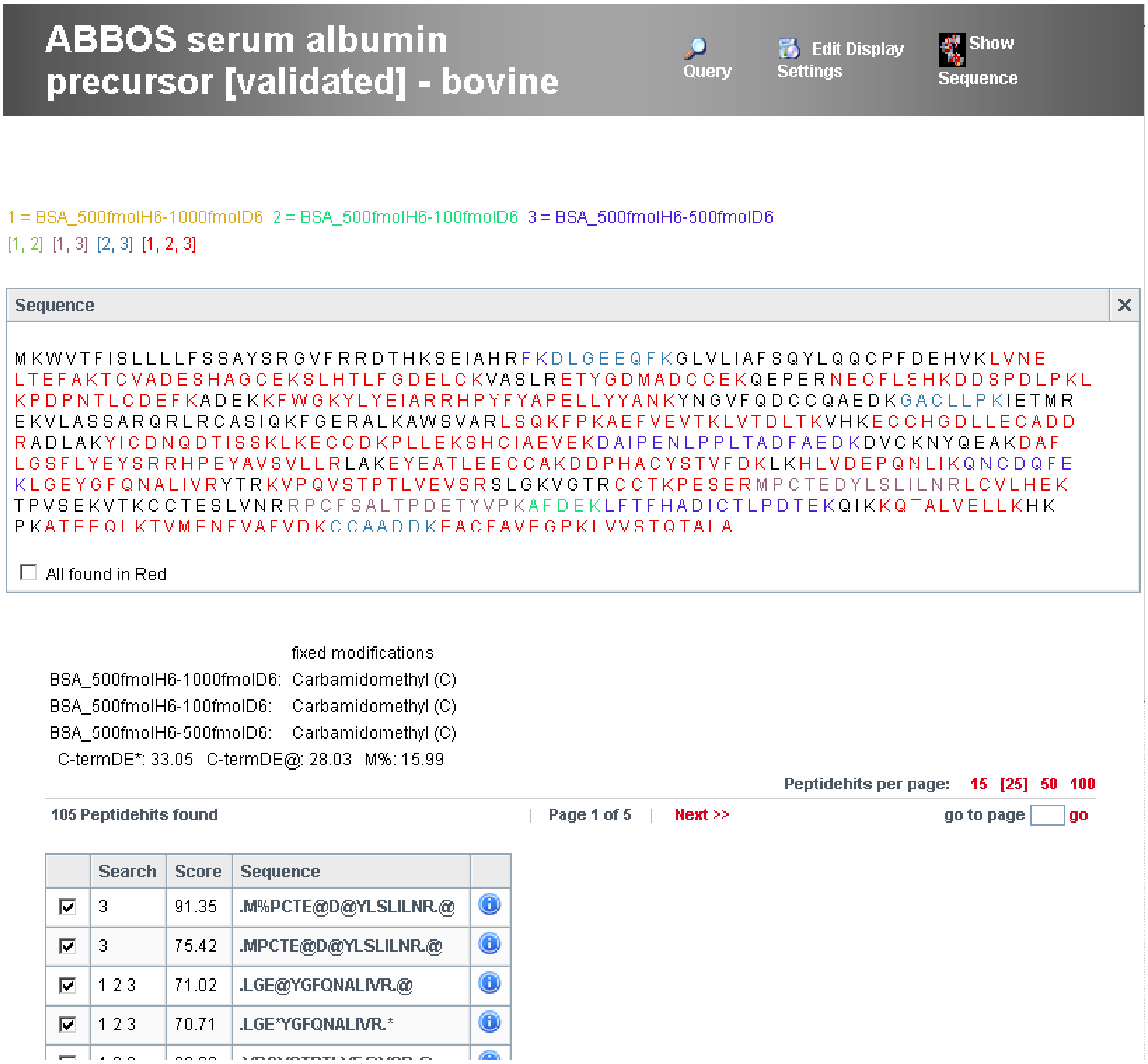


```
                                       400       410       420       430       440       450       460       470       480       490
id|3|maspectras|264353|score|4/1-78: SRILNEMRDQYEQMAEKNRRD-AETWFLSKTEELNKEVASNSELVQSSRSEVTELRRVLQGLEIELQSQLSMKASLENSLEETKGRYCMQLSQIQG-
id|4|maspectras|264354|score|1/1-78: SRILNEMRDQYEKMAEKNRKD-AEEWFFTKTEELNREVATNSELVQSGKSEISELRRTMQNLEIELQSQLSMKASLENSLEETKGRYCMQLAQIQE-
id|29|maspectras|264385|score|/1-78: SRILNEMRDQYEKMAEKNRKD-AEDWFFSKTEELNREVATNSELVQSGKSEISELRRTMQALEIELQSQLSMKASLEGNLAETENRYCVQLSQIQG-
id|10|maspectras|264363|score|/1-78: AKILTDMRSQYEAMVEKNRSD-AEAWFTSKTDELNQEVAVHTKLLQTSKTEVTDLRRTLQGLEIELQSQLSMKAALEGTLAETEARYGVQLSQIQA-
id|12|maspectras|264364|score|/1-78: TQLLNNMRSQYEQLAEQNRKD-AEAWFNEKSKELTTEIDNNIEQISSYKSEITELRRNVQALEIELQSQLALKQSLEASLAETEGRYCVQLSQIHA-
id|8|maspectras|264360|score|1/1-78: DSIIAEVKAQYEEIANRSRTE-AESWYQTKYEELQQTAGRHGDDLRNTKHEISEMNRMIQRLRAEIDNVKKQCANLQNAIADAEQRGELALKDARN-
id|34|maspectras|264386|score|/1-78: PAIISSSNSNKNENAVSTDTS-TPAAAGAPEGKPPQKTSKNKKSLSSKEAQIEELKKFSEKFKVPYDIPKDMLEVLKRSSSTLKSNSSLPPKPISKT
id|21|maspectras|264373|score|/1-78: SVLLRLAKEYEATLEECCAKDDPHACYSTVFDKLKHLVDEPQNLIKQNCDQFEKLGEYGFQNALIVRYTRKVPQVSTPTLVEVSRSLGKVGTRCCTK
id|38|maspectras|264357|score|/1-78: TLGIKGKNLYLSCVMKDNTPT------------LQLEDIDPKRYPKRDMEKRFVFYKTEIKNRVEFESALYPNWYISTSQAEQKPVFLGN-------

                        Conservation 437+433736343533363 36-1001100000264333323336265624263338374344437366345253335436537543343430001 00-
                             Quality
                           Consensus
                                     SRILNEMR+QYE+MAEKNRKD-AEAWFF+KTEELNQEVATNSEL+QS+KSEI+ELRRT+Q+LEIELQSQLSMKASLENSLAET+GRYCVQLSQIQ+-
```



7.3 Peptide comparison:



1 = BSA_500fmolH6-1000fmolD6 2 = BSA_500fmolH6-100fmolD6 3 = BSA_500fmolH6-500fmolD6
[1, 2] [1, 3] [2, 3] [1, 2, 3]

Sequence

MKWVTFISLLLLFSSAYSRGVFRRDTHKSEIAHRFKDLGEEQFKGLVLIAFSQYLQQCPFDEHVKLVNE
LTEFAKTCVADESHAGCEKSLHTLFGDELCKVASLRETYGDMADCCEKQEPERNECFLSHKDDSPDLPKL
KPDPNTLCDEFKADEKKFWGKYLYEIARRHPYFYAPELLYYANKYNGVFQDCCQAEDKGACLLPKIETMR
EKVLASSARQRLRCASIQKFGERALKAWSVARLSQKFPKAEFVEVTKLVTDLTKVHKECCHGDLLECADD
RADLAKYICDNQDTISSKLKECCDKPLLEKSHCIAEVEKDAIPENLPPLTADFAEDKDVCKNYQEAKDAF
LGSFLYEYSRRHPEYAVSVLLRLAKEYEATLEECCAKDDPHACYSTVFDKLKHLVDEPQNLIKQNCDQFE
KLGEYGFQNALIVRYTRKVPQVSTPTLVEVSRSLGKVGTRCCTKPESERMPCTEDYLSLILNRLCVLHEK
TPVSEKVTKCCTESLVNRRPCFSALTPDETYVPKAFDEKLFTFHADICTLPDTEKQIKKQTALVELLKHK
PKATEEQLKTVMENFVAFVDKCCAADDKEACFAVEGPKLVVSTQTALA

☐ All found in Red

	fixed modifications
BSA_500fmolH6-1000fmolD6:	Carbamidomethyl (C)
BSA_500fmolH6-100fmolD6:	Carbamidomethyl (C)
BSA_500fmolH6-500fmolD6:	Carbamidomethyl (C)

C-termDE*: 33.05 C-termDE@: 28.03 M%: 15.99

Peptidehits per page: 15 [25] 50 100

105 Peptidehits found | Page 1 of 5 | Next >> go to page ☐ go

	Search	Score	Sequence	
☑	3	91.35	.M%PCTE@D@YLSLILNR.@	ⓘ
☑	3	75.42	.MPCTE@D@YLSLILNR.@	ⓘ
☑	1 2 3	71.02	.LGE@YGFQNALIVR.@	ⓘ
☑	1 2 3	70.71	.LGE*YGFQNALIVR.*	ⓘ

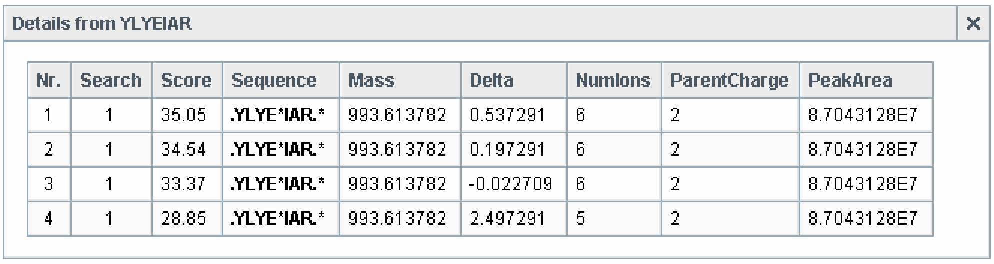
At the header the gene-name is indicated. The button brings the box with the protein sequence if you have closed it. Below the header the searches are listed again, this time in colour in order to recognize them in the protein sequence. Underneath the possible combinations of the searches are colour-encoded as well.
The “Sequence” box has a little checkbox “All found in Red”. With this box you can show all found parts of the sequence in red, if one colour is not so well visible for you.
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.
Then the found peptides are listed, sorted by the score by default. To indicate in 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 the peptide this peptide will be removed as found in the “Sequence” box.

When you push the blue ⓘ button you get detailed information about this 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.@		ⓘ

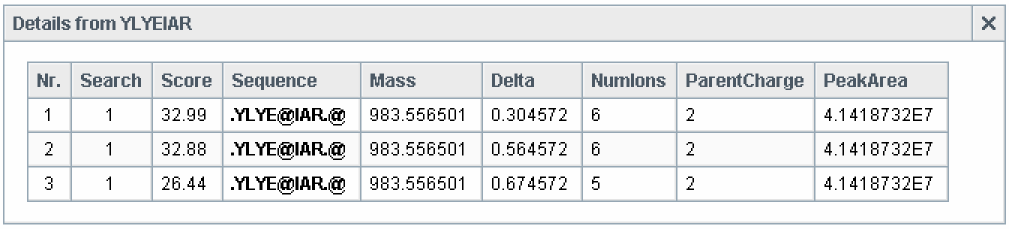
Peptidehits per page: [15] 25 50 100

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

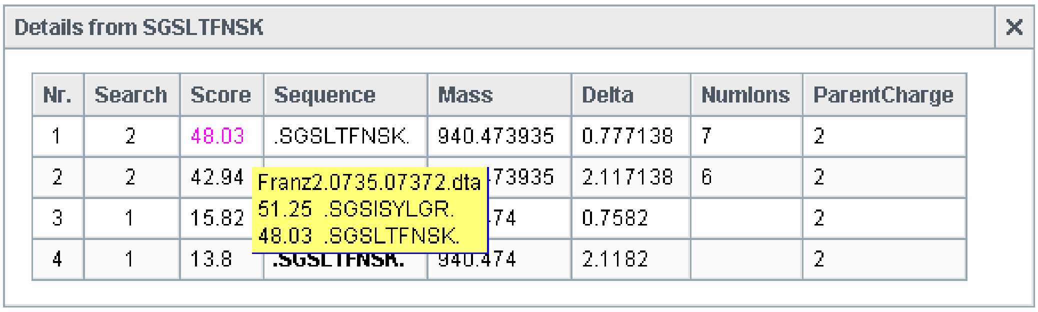


Details from YLYEIAR

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 hover your mouse above one entry of the column “Search”, “Sequence” or “Score” a tooltip with the hits will be displayed.



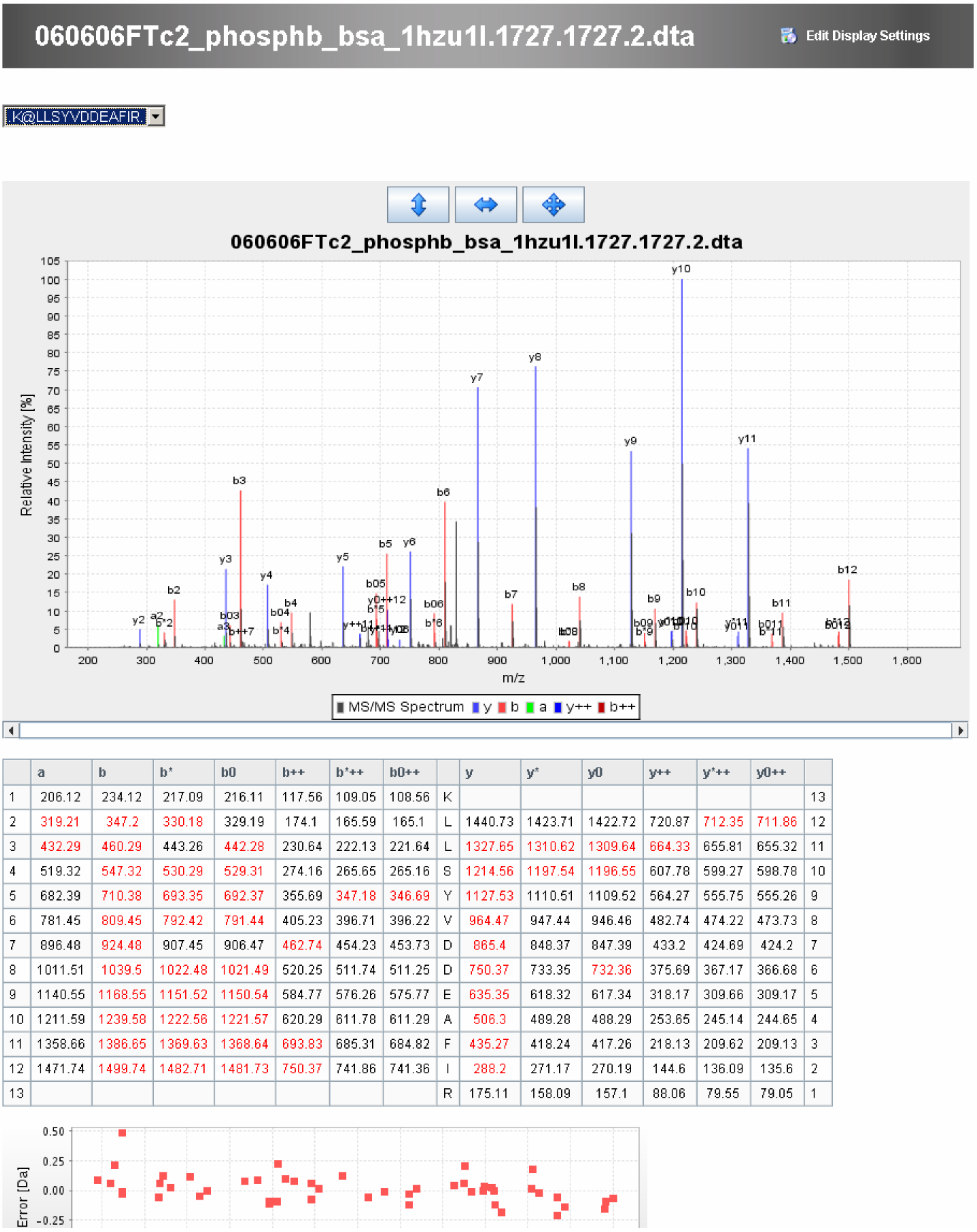
Details from SGSLTFNSK

Nr.	Search	Score	Sequence	Mass	Delta	NumIons	ParentCharge
1	2	48.03	.SGSLTFNSK.	940.473935	0.777138	7	2
2	2	42.94		73935	2.117138	6	2
3	1	15.82		74	0.7582		2
4	1	13.8	**.SGSLTFNSK.**	940.474	2.1182		2

Franz2.0735.07372.dta
51.25 .SGSISYLGR.
48.03 .SGSLTFNSK.

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:



060606FTc2_phosphb_bsa_1hzu1l.1727.1727.2.dta

K@LLSYVDDEAFIR

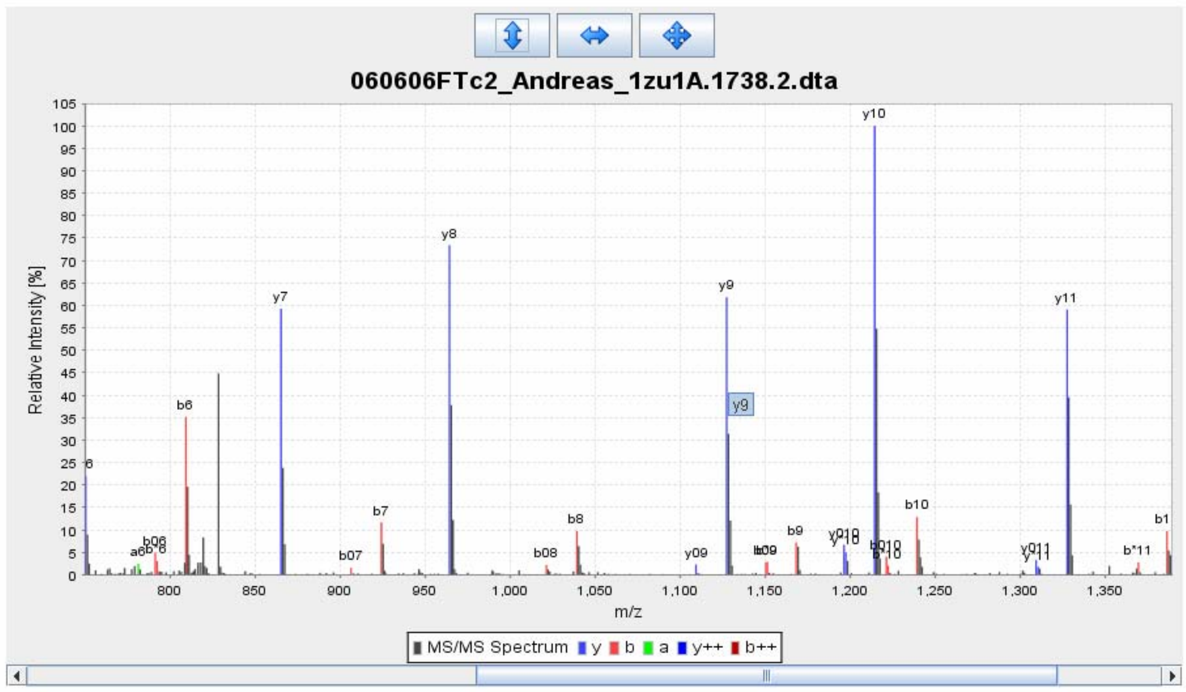
060606FTc2_phosphb_bsa_1hzu1l.1727.1727.2.dta

MS/MS Spectrum ▮ y ▮ b ▮ a ▮ y++ ▮ b++

	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 have 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:



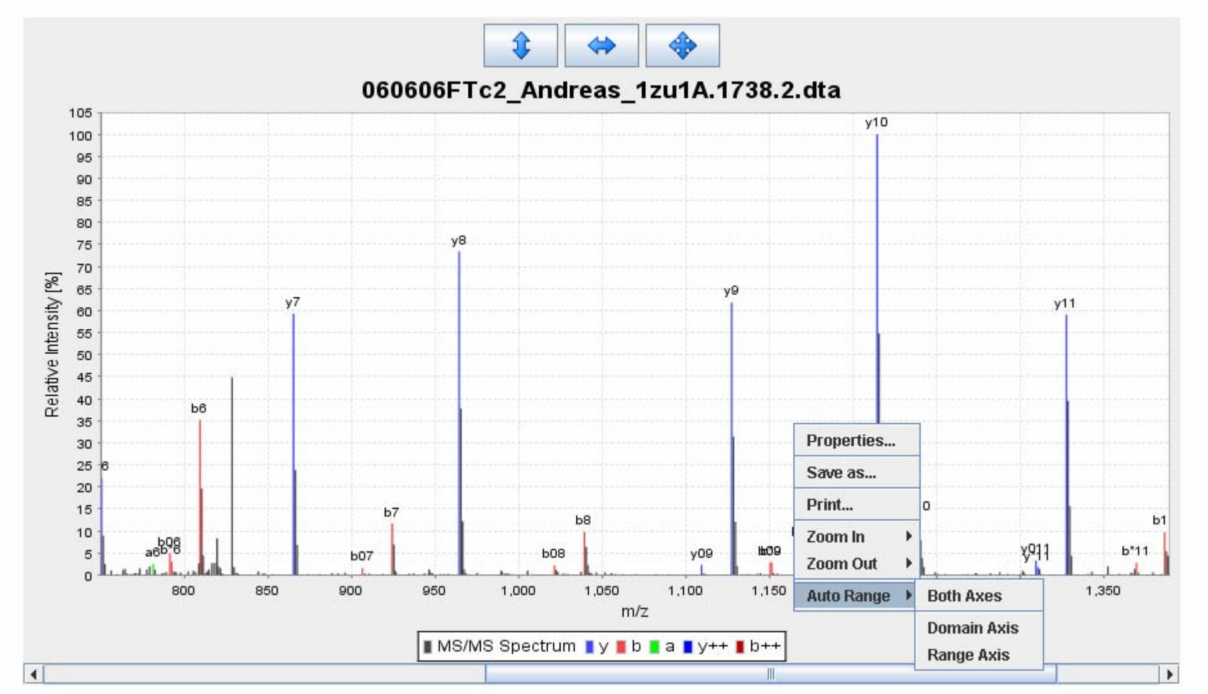
The not assigned peaks are displayed in red. The assigned fragment name is written on the top of the peak. If you hover your mouse above one peak the name will be displayed in a tooltip as well. You can zoom into your spectrum and scroll the x-axis with the bar at the bottom.

↕ : 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.

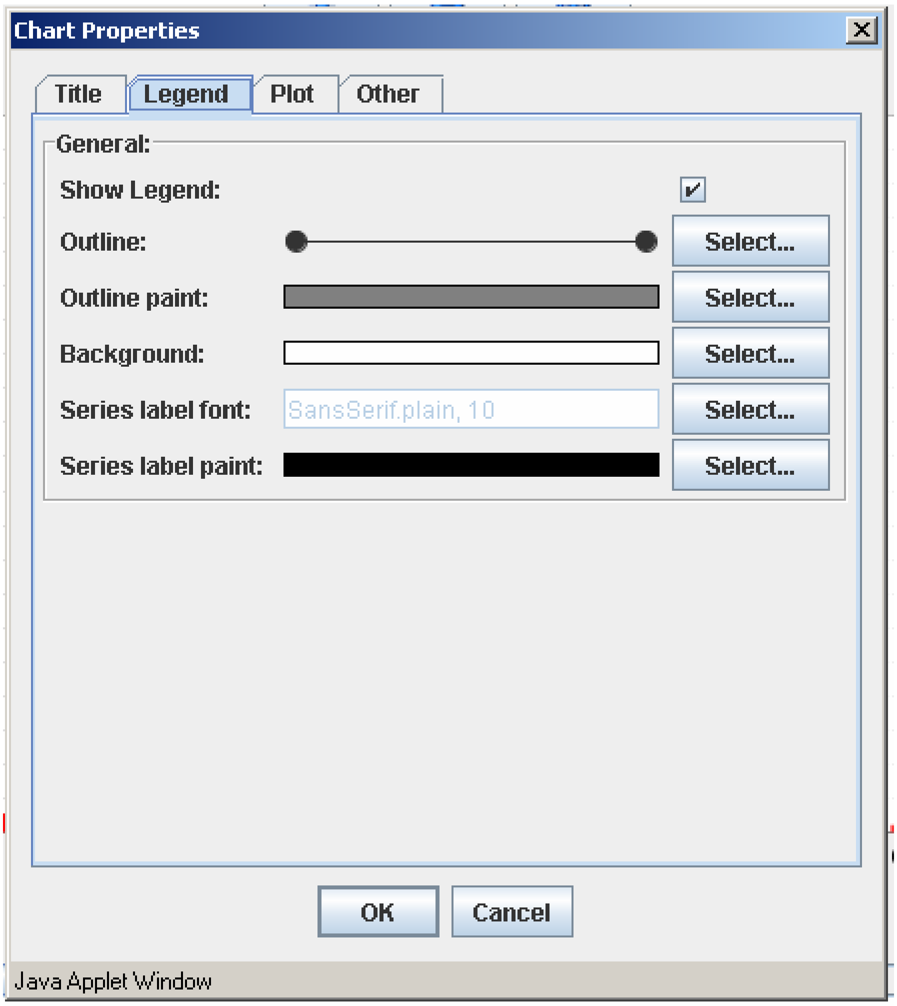


Chart Properties

General:

Show Legend: ☑

Outline:

Outline paint:

Background:

Series label font: SansSerif.plain, 10

Series label paint: