

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:

Bioinformatics Graz **maspectras**
MAAss SPECTRometry Analysis System

Home login | please login

MASPECTRAS
MAAss SPECTRometry Analysis System

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Release Information:
VersionAlpha 0.1
Build 20050826

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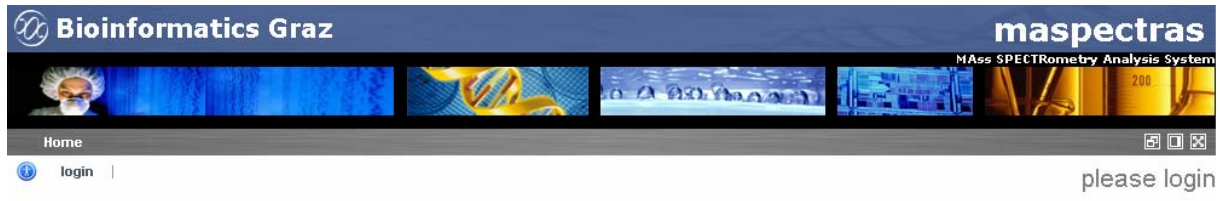
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This will be your first impression of MASPECTRAS.
The main view is divided into 3 sections:

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:



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:

change your password

	username:	<input type="text" value="hartler"/>
	Fullname:	<input type="text" value="Juergen Hartler"/>
	old password	<input type="password"/>
	new password	<input type="password"/>
	repeat new password	<input type="password"/>
		<input type="button" value="Submit"/> <input type="button" value="Cancel"/>

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:

Protein



Query



Edit Display Settings

1 = SpectrumMill (Partitioning )

Proteins per page: **[15]** 25 50 100

107 Proteins found

<< Previous | Page 2 of 8 | Next >>

go to page go

Nr.	AccessionNum	GeneName	SequCovMax
16	gil15237374	NP_199421 expressed protein [Arabidopsis thaliana].	11.214953271028037
17	gil30962111	albumin [Felis catus]	11.13013698630137
18	gil2108238	HFLK homolog [Treponema pallidum]	10.909090909090908
19	gil24213640	NP_711121 hypothetical protein LA0940 [Leptospira interrogans serovar Lai str. 56601].	10.204081632653061
20	gil113578	ALBU_PIG Serum albumin precursor	10.082644628099173
21	gil3319897	albumin [Canis familiaris]	9.572649572649574
22	gil23028929	COG0637: Predicted phosphatase/phosphohexomutase [Microbulbifer degradans 2-40]	9.502262443438914
23	gil17536277	NP_495370 putative N-myristoylated protein (2H10) [Caenorhabditis elegans].	9.210526315789473
24	gil6687188	AJ133489_1 Canis familiaris mRNA for serum albumin.	9.210526315789473
25	gil23098581	hypothetical protein OB1126 [Oceanobacillus ihayensis HTE831]	9.174311926605505
26	gil2492797	ALBU_MACMU Serum albumin precursor	8.833333333333334
27	gil121697	GST26_SCHJA Glutathione S-transferase 26 kDa (GST 26) (SJ26 antigen) (GST class-mu)	8.715596330275229
28	gil84402	A26484 glutathione transferase (EC 2.5.1.18) - fluke (Schistosoma japonicum) (fragment)	8.67579908675799
29	gil22987378	COG4791: Type III secretory pathway, component EscT [Burkholderia fungorum]	8.656716417910449
30	gil595718	glutathione S-transferase	8.189655172413794

Proteins per page: **[15]** 25 50 100

107 Proteins found

<< Previous | Page 2 of 8 | Next >>

go to page go

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:

Query

Masc/+1 Score

>

20

×

Masc/+2 Score

>

25

×

Masc/+3 Score

>

30

×

SMill/+1 Score

>

15

×

SMill/+2 Score

>

18

×

SMill/+3 Score

>

22

×

AND

Submit Query

Reset Query

Restore Default

Save 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:

Available fields					X
Required Information					
<input checked="" type="checkbox"/> AccessionNum	<input type="checkbox"/> Organism	<input type="checkbox"/> Sequence	<input type="checkbox"/> PredictedPi	<input type="checkbox"/> Nr. of Proteins	
<input checked="" type="checkbox"/> GeneName	<input type="checkbox"/> OrfNumber	<input type="checkbox"/> Modifications	<input checked="" type="checkbox"/> SequCovMax	<input type="checkbox"/> Cluster Nr.	
<input type="checkbox"/> Synonyms	<input type="checkbox"/> Description	<input type="checkbox"/> PredictedMass	<input type="checkbox"/> Score	<input type="checkbox"/> Search	
Update Display all Display default					Save Settings

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:



Sharing



You are about to share item: **quantTest.June2006**

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

	Name	Full Name	E-Mail	
<input type="checkbox"/>	 hartler	Juergen Hartler	juergen.hartler@tugraz.at	 <input type="checkbox"/>  <input type="checkbox"/>
<input type="checkbox"/>	 testmaspectras	Test Maspectras	juergen.hartler@tugraz.at	 <input type="checkbox"/>  <input type="checkbox"/>
<input type="checkbox"/>	 stocker	Gernot Stocker	gernot.stocker@tugraz.at	 <input type="checkbox"/>  <input type="checkbox"/>
<input type="checkbox"/>	 mechtler	Karl Mechtler	Karl.Mechtler@imp.univie.ac.at	 <input type="checkbox"/>  <input type="checkbox"/>


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:




lonsource: 

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”.


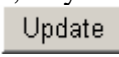

1.2.5 Multiple input Fields and other buttons:

Detection Agents: 


Detection Agent:   



Detection Agent:   


Add detection agent



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  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.



Rehydration solutions: 

Rehydration solution:  

 Details for gel matrix 	
Component	Concentration
componentOne	1.0
componentTwo	2.0

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.

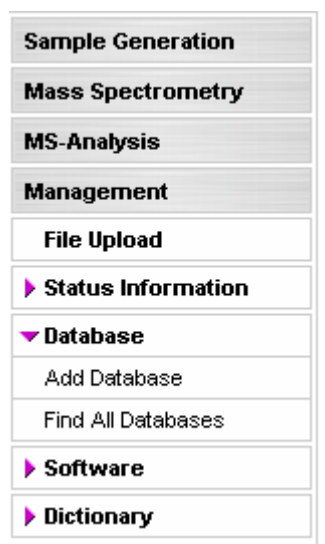
 **Rehydration solution** 

The components, with concentrations (excluding the sample) of the rehydration solution which is loaded onto the gel, if appropriate.

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.

New Database


Databasename:	<input type="text"/>
Version:	<input type="text"/>
File	<input type="text"/> <input type="button" value="Browse..."/>
Description:	<div><div></div></div>

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:	<input type="text" value="(gi \d+)\\"/>
Rule to parse description string from Fasta file:	<input type="text" value="[^\]* (.*)"/>
Rule to parse organism from Fasta file:	<input type="text" value="[^\]*([^\w\s]+\s)+\\"/> .*

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

[Return](#)

[Add Version](#)

At the top you can define your parsing rules for the accession string, the description string and the organism string. Examples for parsing rules you will find in your installation package at </doc/parsingRules>. The meaning for the regexs you can find at <http://java.sun.com/j2se/1.5.0/docs/api/java/util/regex/Pattern.html>. 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]Ogi|1723488|sp|Q103:
MRSYSNPENGGQINDNINYSERPTMLPENLSLSNYDMDSFLGQFPDNNMQLPSTYEQHLQGEQQNPTNPNYFPPEFD
ENKVDWKQEKPKPDAPSFADNNSFDNNSKLTNPSPVQPNIVKSESEFANSKQNEVVEATSVKAKENVVAHESGTPESG
GSTSAPKSKKQRLTADQLAYLLREFSKDTNPPPAIREKIGRELNIPERSVTIWFQNRRAKSKLISRRQEEERQILREQR
ELDSLQKVSQAFAHEVLSTSPYVGGIAANRQYANTLLPKPTRKTGNFYMKSGPMQSSMEPCIAESDIPIRQSLST
YNSLSLSPNAVPSQKRYASSYSAIPNAMSVSNOAFDVESPPSYATPLTGIRMPQESDLYSYPREVSPSSGGYRMFG
HSPKSSYKASGPPRPPNMTAGHMTSSEPTSYDSEFYFSCSTLLVIGLWKRLRASPDLMCFYSPPKKLFAYLIQFQGIQ
YRIEYFFVIESIHVFRVEEPLNELSATASSRDKPAPNEYWLQMDIQLSVPPVPHMITSEGGNCDFTEGNQASEVLL
HSLMGRATSMFQMLDRVRASPELGSVIRLQKGLNPHQFLDPQWANQLPRQPDSSVFDHQRNPPIQGLSHDTSSEYGNK
SQFKRLRSTSTPARQDLAHLPLPKTNTTEGLMHAQSVSPITQAMKSANVLEGSSTRLNSEYSPSSATPHHNLALNLDNT
QFGEIGTNSIYPLSAPSDVGLSPRASNSPSRPVMPHNTQGINTEIKDMAAQFPNSQTGGLTPNSWSHNTNVSPFTTQN
REFGGIGSSSISTTNNAPSQQLSQVPGDVSLATENSVPYGFVPESESVYAQARTNSSVSAGVAPRLFIQTPSIPLAS
SAGQDSNLIEKSSGGVYASQPGASGYLSDHDSGSPFEDVYSPSAGIDFQKLRGQFSPDMQ

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]
MPFSFLAQFPFPCKISSTHSLGVNSPGRGSHGNLNVFYKLSISGLIEEDIVVDSPGFVVISLLLLWLVGVGLLILVLPV
AFVPGFATVVPILKLENVFLGDIUFVVDVGLDSSDVLSSIVFIPGL

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]Ogi|170991:
MGKYTKTAILSVYDKTGLLDLAKGLVENNVRLASGGTANMVREAGFPVDDVSSITHAPEMLGGRVKTLLHPAVHAGILAR
NLEGEKDLKEQHIDKVDVFCNLYPFKETAIGVTVQEAEEIDIGGVTLRLAAKNHRSVITLSDPNDYSIFLQDLS
KDGEISQDLNRFALKAFETADYDAISDFFRKQYSEKQAQLPLRYGCNPHQRPAQAYITQEEELPFKVLCTPGYINL
LDALNSUPLVKELASLNLPAASFKHVPAGAAVGLPLSDVERQVYFVNDMEDLSPLACAYARAGADRMSFFGDFIAL
SNIVDVATAKIIKSEKVDGVIAPGYEPEALNLSKKKNGKYCILQIDPNYVPGMESREVFVGTLLQQRNDAIINQSTFK
EIVSKNKALTEQAVIDLTVATLVKLKYTQSNVCAKNGMVVGLGAGQQSRIHCTRLAGDKTDNWWLRQHPKVLNMKWAQK
IKRADKSNALDLFVVTGQRIEGPEKVDYESKFEVPEPFTKEERLEWLSKLNVSLSDDAFFFPDNNVYRAVQSGVKFITA
PSGSVMDDKVVFAADSFDIVYVENPIRLFHH

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)
- 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:

Sample Generation
Mass Spectrometry
MS-Analysis
Management
File Upload
► Status Information
► Database
► Software
► Dictionary

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

File Upload

Query
 Edit Display Settings

29 Files found

Page 1 of 2 | [Next >>](#)

Files per page: [\[15\]](#) [25](#) [50](#) [100](#)

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				

29 Files found

Page 1 of 2 | [Next >>](#)

Files per page: [\[15\]](#) [25](#) [50](#) [100](#)

go to page [go](#)

New file upload

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

New File Upload

Name		
File	<input type="text"/>	Browse...
File Type		
Comment	Raw-File SpectrumMill SpectrumMill Before Version A.03.02 SM Config SM Custom Config Mascot Sequest XITandem Omssa Omssa Modification File	
Upload		

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.

Sample Generation
Management
File Upload
▼ Status Information
Upload Status

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

Upload Status

	ID	Upload Name	Status	Step	Progress	in %
<input type="checkbox"/>	11850	testKarl1	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	11851	testKarl22	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	11852	testKarl23	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	11951	F001244	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	12050	F001276	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	13000	Task1ms22400-3600	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	13300	SpectrumMill	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	13301	MascotCompSpectrMill	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	13400	BSA_500fmolIH6-1000fmolD6	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	13550	CompToSequest	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	14250	Task2synthDBAll	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	14350	Task2testKarlDB2	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	14450	newMascot	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	14750	MSDB	LOADING FINISHED		<div></div>	100 %
<input type="checkbox"/>	14850	Task2CompToMasc	LOADING FINISHED		<div></div>	100 %

Update Interval [m:ss]

Select All

Select Finished

Select Failures

Invert Selection

Delete Selected

2.4 Software:





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

Sample Generation
Mass Spectrometry
MS-Analysis
Management
File Upload
► Status Information
► Database
▼ Software
Add Software
Find All Softwares
► Dictionary

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.



New Software




Name:	<input type="text"/>	
Version:	<input type="text"/>	
DateOfRelease:	<input type="text"/>	
Role:	<input type="text"/>	
Upgrades		
Upgrade:	<input type="text"/>	
Add Upgrade		
<input type="button" value="Create"/>		

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

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

Software

 Query  Edit Display Settings

1 Softwares found				Page 1 of 1		Softwares per page: 15 [25] 50 100		go to page <input type="text"/> go
Nr.	Name	Version	Role					
1	XCalibur	2.0	massSpectrometrySoftware					
1 Softwares found				Page 1 of 1		Softwares per page: 15 [25] 50 100		go to page <input type="text"/> go

2.5 Dictionary:

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

Sample Generation
Mass Spectrometry
MS-Analysis
Management
File Upload
► Status Information
► Database
► Software
▼ Dictionary
Add Dictionary
Find All Dictionarys

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.

New MaspectrasDictionary

Domain:	<input type="text"/>
Value:	<input type="text"/>
Description:	<input type="text"/>

Create

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

MaspectrasDictionarys per page: **15** [25] 50 100

43 MaspectrasDictionarys found

Page 1 of 2 | [Next >>](#)

go to page [go](#)

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-hydroxycinnamic 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.

Sample Generation
Sample Processing
Mass Spectrometry
MS-Analysis
Management
File Upload
► Status Information
► Database
► Software
▼ Equipment
Add Equipment
Find All Equipments
► Dictionary

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.

New Equipment

ModelName:	<input type="text"/>
EquipmentType:	<input type="text" value="gelTank"/> 
ModelManufacturer:	<input type="text"/> 
ModelNumber:	<input type="text"/>

Create

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.

Equipment



















 Query  Edit Display Settings

Equipments per page: 15 [25] 50 100

6 Equipments found

Page 1 of 1

go to page go

Nr.	ModelName			
1	anotherEquipment			
2	laserScannerEquipment			
3	testAdding			
4	testInterAdding			
5	testOneMoreAdding			
6	bufferEquipment			

Equipments per page: 15 [25] 50 100

6 Equipments found

Page 1 of 1

go to page go

3. Sample Description:

3.1 Experiment:

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

Sample Generation
▼ Experiment
Add Experiment
Find All Experiments
▶ Sample
▶ Sampleorigin
▶ Organism
▶ Taggingprocess
Mass Spectrometry
MS-Analysis
Management

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

New Experiment

Hypothesis:

MethodCitations:






ResultCitations:

Title:

Description:

Create

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

Experiment					 Query	 Edit Display Settings
1 Experiments found					Experiments per page: 15 [25] 50 100	
Page 1 of 1					go to page <input type="text"/> go	
Nr.	Title					
1	testExp					
1 Experiments found					Experiments per page: 15 [25] 50 100	
Page 1 of 1					go to page <input type="text"/> go	

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.

Sample Generation
▶ Experiment
▼ Sample
Add Sample
Find All Samples
▶ Sampleorigin
▶ Organism
▶ Taggingprocess
Mass Spectrometry
MS-Analysis
Management

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

New Sample

SampleId:	<input type="text"/>
SampleDate:	<input type="text"/> 
Title:	<input type="text"/>
ProteinAmount:	<input type="text"/>
Description:	<div><div></div></div>

Sampleorigins	
Sampleorigin:	<div><div></div><div></div><div></div></div>  
Add Sampleorigin	

Create

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 “Sampleorigin”.

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

Sample

[Query](#)[Edit Display Settings](#)

Samples per page: 15 [25] 50 100

4 Samples found

Page 1 of 1

go to page go

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					

Samples per page: 15 [25] 50 100

4 Samples found

Page 1 of 1

go to page go

3.2.2 Sample over experiment:

Experiment

[Query](#)[Edit Display Settings](#)

Experiments per page: 15 [25] 50 100

1 Experiments found

Page 1 of 1

go to page go

Nr.	Hypothesis	Title	Submitter			
1	testExp	testExp	Juergen Hartler			

Experiments per page: 15 [25] 50 100



1 Experiments found

Page 1 of 1

go to page go

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.

Sample







 Query  Edit Display Settings

Samples per page: 15 [25] 50 100

2 Samples found

Page 1 of 1

go to page go

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

Samples per page: 15 [25] 50 100

2 Samples found

Page 1 of 1

go to page go

[Return](#)

[Create Sample for Experiment](#)


[Add Samples](#)

[Compare Results](#)

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.

New Sample

SampleId:	<input type="text"/>
SampleDate:	<input type="text"/> 
Title:	<input type="text"/>
ProteinAmount:	<input type="text"/>
Description:	<input type="text"/>

Add Sampleorigin

[Return](#)

[Create](#)

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

Experiment: **testExp** ID: 300

Sample

Query
Edit Display Settings

Samples per page: 15 [25] 50 100

2 Samples found | Page 1 of 1 | go to page go

SampleId
<input type="checkbox"/> testQuanti
<input type="checkbox"/> testProphetScore

> >
< <

Samples per page: 15 [25] 50 100

2 Samples found | Page 1 of 1 | go to page go

SampleId
<input type="checkbox"/> forLexi
<input type="checkbox"/> newMascot

Samples per page: 15 [25] 50 100

2 Samples found | Page 1 of 1 | go to page go

Samples per page: 15 [25] 50 100

2 Samples found | Page 1 of 1 | go to page go

Return

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->Sampleorigin you reach the sample origin section.

Sample Generation

▶ Experiment

▶ Sample

▼ Sampleorigin

Add Sampleorigin
Find All Sampleorigins

▶ Organism

▶ Taggingprocess












Mass Spectrometry

MS-Analysis

Management

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

New Sampleorigin

Name:		
Organism:	<input type="text"/>	
Taggingprocess:	<input type="text"/>	
Condition:	<input type="text"/>	
ConditionDegree:	<input type="text"/>	
Environment:	<input type="text"/>	
TissueType:	<input type="text"/>	
CellType:	<input type="text"/>	
CellCyclePhase:	<input type="text"/>	
CellComponent:	<input type="text"/>	
Technique:	<input type="text"/>	
MetabolicLabel:	<input type="text"/>	
Description:	<div><div></div></div>	
<div>Create</div>		

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:

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

Nr.	Name	Organism			
1	aGoodOrigin	Human			

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

3.4 Organism:

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

Sample Generation

▶ Experiment

▶ Sample

▶ Sampleorigin

▼ Organism

Add Organism

Find All Organisms

▶ Taggingprocess

Mass Spectrometry

MS-Analysis

Management

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

New Organism

SpeciesName:	<input type="text"/>
StrainIdentifier:	<input type="text"/>
RelevantGenotype:	<input type="text"/>

Create

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

Organism

Query
 Edit Display Settings

1 Organisms found

Page 1 of 1

Organisms per page: 15 [25] 50 100

go to page go

Nr.	SpeciesName			
1	Human			

1 Organisms found

Page 1 of 1

Organisms per page: 15 [25] 50 100

go to page go

3.5 Taggingprocess:

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

Sample Generation

▶ Experiment

▶ Sample

▶ Sampleorigin

▶ Organism

▼ Taggingprocess

Add Taggingprocess

Find All Taggingprocesses



Mass Spectrometry

MS-Analysis

Management

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

New Taggingprocess

Name:	<input type="text"/>
LysisBuffer:	<input type="text"/> 
TagType:	<input type="text"/> 
TagPurity:	<input type="text"/>
ProteinConcentration:	<input type="text"/>
TagConcentration:	<input type="text"/>
FinalVolume:	<input type="text"/>
IncubationTime:	<input type="text"/>

Create

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

Taggingprocess

 Query  Edit Display Settings

1 Taggingprocesss found

Page 1 of 1

Taggingprocesss per page: 15 [25] 50 100 go to page go

Nr.	Name			
1	myTaggingProcess			

1 Taggingprocesss found

Page 1 of 1



Taggingprocesss per page: 15 [25] 50 100 go to page go

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:

Sample













 Query  Edit Display Settings

Samples per page: 15 [25] 50 100

4 Samples found

Page 1 of 1

go to page go

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					

Samples per page: 15 [25] 50 100

4 Samples found

Page 1 of 1

go to page go

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:

Tree View

Sample testSample

 Edit Display Settings

refresh tree

Sample

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

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:

Tree View

Sample quantificationApril2006

Edit Display Settings

refresh tree

Sample

MS Experiment

Gel 2D

Spot

MS Experiment

Chemical Treatment

Treated Analyte

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 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:

Tree View

Sample testSample

Edit Display Settings

refresh tree

Sample

Lc Column

Fraction

Fraction

Fraction

Chemical Treatment

Treated Analyte

Gel 2D

Spot

Spot

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. 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:

Tree View

refresh tree

Sample

Lc Column

Fraction

Fraction

Fraction

Chemical Treatment

Treated Analyte

Gel 2D

Spot

Spot

Treated Analyte myTreatedSample

Edit Display Settings

Gel 1D

add Gel 1D

Gel 2D

Nr.	Description	PercentAcrylamide	StainDetails	PiStart	PiEnd	MassStart	MassEnd		
1	myGel2dExperiment								

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

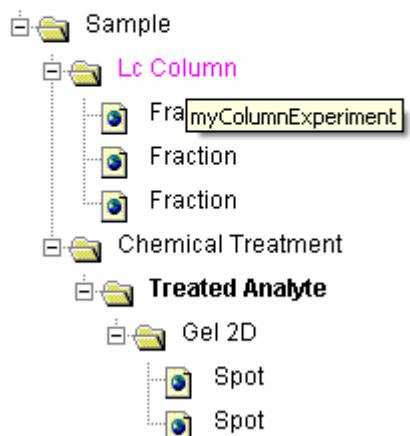
There are 5 different processing methods. A Gel1D leads to bands (for detailed information see chapter 4.2 Gel1D), a Gel2D leads to spots (for detailed information see chapter 4.3 Gel2D), a LC-Column leads to Fractions (for detailed information see chapter 4.4 LC-Column), a Chemical Treatment leads to 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.

Tree View

refresh tree



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:

Sample testSample

 Edit Display Settings

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Other analyte 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 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.

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 can edit it again.




Edit Gel1D
Edit Display Settings

Gel1DId:
testFull

Gel
Buffer
Band Detection
Image Acquis.
Image




Acquisition Equipments:
?




Acquisition Equipment:
laserScannerEquipment




Acquisition Equipment:
anotherEquipment




Add equipment

Acquisition Softwares:
?

Acquisition Software:
imageAcquSoftware 1.0 2 Softwareupgrar




Acquisition Software:
anotherSoftwareType 2.0




Add image acquisition softwares

EquipmentCalibration:
manual
?





EquipmentSpecificParams:
EquipmentSpecificParams
?

ImageAcquisitionProcess:
ImageAcquisitionProcess
?

Acquisition Component:
stacking gel x:6.0 y:7.0 z:8.0
?

Update

add Band

Nr.	Title	Area	Intensity	LocalBackground	Annotation	Normalisation	Description		
1	test	1.0	2.0	3.0	4	aNormalizationMethod	dasd		
2	testBoundaryChain								

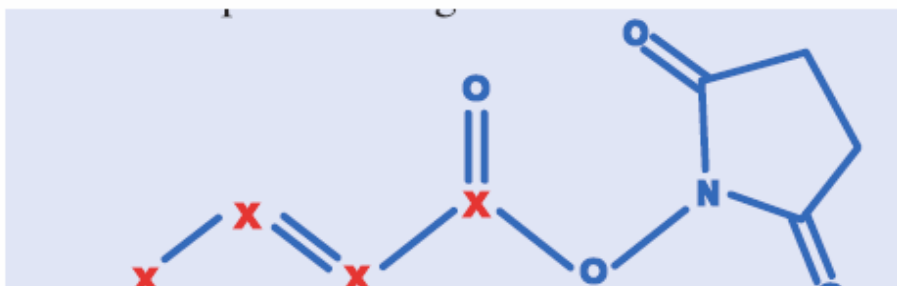
For the “Acquisition Component” you can select the whole selected “Gelmatrix” named with “Main” (you will find this select field, when you click on the “Gel” tab) or one of the components of the “Gelmatrix”. The references to the files (mostly images) which you can select in the “Image” tab, must be 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).

Edit Band

Title:	<input type="text" value="testBoundaryChain"/>			
Area:	<input type="text"/>		?	
Intensity:	<input type="text"/>		?	
LocalBackground:	<input type="text"/>		?	
Annotation:	<input type="text"/>		?	
AnnotationSource:	<input type="text"/>		?	
Volume:	<input type="text"/>		?	
Normalisation:	<input type="text"/>	<input type="radio"/>	?	
NormalisedVolume:	<input type="text"/>		?	
LaneNumber:	<input type="text"/>		?	
ApparentMass:	<input type="text"/>		?	
Description:	<div><div></div></div>		?	
LocalisationItemType:	<input type="text" value="Boundary Chain"/>			
Boundarypoints:	?			
X:	<input type="text" value="1.0"/>	Y:	<input type="text" value="2.0"/> ?	
Directionstep:	<input type="text" value="NE"/>	<input type="text" value="14"/>	[pxs] X	
Directionstep:	<input type="text" value="SW"/>	<input type="text" value="16"/>	[pxs] X	

Add direction step



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:

LocalisationItemType:	Rectangle		
X-Coordinate:	<input type="text"/>	[px]	?
Y-Coordinate:	<input type="text"/>	[px]	?
X-Size:	<input type="text"/>	[pxs]	?
Y-Size:	<input type="text"/>	[pxs]	?

Boundary points:

LocalisationItemType:	Boundary Points					
Boundarypoints:	?					
X:	<input type="text"/>	[px]	Y:	<input type="text"/>	[px]	×
X:	<input type="text"/>	[px]	Y:	<input type="text"/>	[px]	×
X:	<input type="text"/>	[px]	Y:	<input type="text"/>	[px]	×

Add boundary point

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

4.3 Gel2D:

Sample testSample

 Edit Display Settings

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Other analyte 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 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.

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 the “create/edit” page again.

Gel2dd: testlt1

Gel | **Buffer** | **Inter Dim.** | **Spot Detection** | **Image Acquis.** | **Image**

Acquisition Equipments: ?

Acquisition Equipment: laserScannerEquipment ?

Add equipment

Acquisition Softwares: ?

Acquisition Software: anotherSoftwareType 2.0 ?

Add image acquisition softwares

EquipmentCalibration: automatic ?

EquipmentSpecificParams: EquipmentSpecificParams ?

ImageAcquisitionProcess: ImageAcquisitionProcess ?

Acquisition Component: Main Y ?

Update

add Spot

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.

<i>Gel</i>	Buffer	<i>Inter Dim.</i>	<i>Spot Detection</i>	<i>Image Acquis.</i>	<i>Image</i>
Buffer X		Buffer Y			
BufferProtocolY:		BufferProtocolY2			
Running Buffers:		?			
Running Buffer:		anotherBuffer	+	●	×
Running Buffer:		testAdding	+	●	×

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

Title:	testASpot		
Area:	1.5		?
Intensity:	2.0		?
LocalBackground:	3.0		?
Annotation:	Annotation		?
AnnotationSource:	AnnotationSource		?
Volume:	4.0		?
Normalisation:	anotherOne	<input checked="" type="radio"/>	?
NormalisedVolume:	5.5		?
ApparentMass:	6.0		?
ApparentPi:	7.0		?
Description:	<div>Description</div>		
LocalisationItemType:	Boundary Chain		
Boundarypoints:	?		
X:	1.0	Y:	2.0 ?
Directionstep:	SE	3	[pxs] X
Directionstep:	E	4	[pxs] X
Directionstep:	N	6	[pxs] X
Directionstep:	NW	7	[pxs] X
Directionstep:	W	8	[pxs] X
Directionstep:	SW	9	[pxs] X
Directionstep:	S	10	[pxs] X
Add direction step			
<input type="button" value="Update"/>			

albumin [Bos taurus]; albumin [Bos taurus]

 Query

 Edit Display Settings

 Show Sequence

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:

LocalisationItemType:	Circle		
X-Coordinate:	1.0	[px]	?
Y-Coordinate:	2.0	[px]	?
Radius:	3.0	[pxs]	?

Boundary points:

LocalisationItemType:		Boundary Points		
Boundarypoints:				
X:	1.0	[px]	Y:	2.0
				[px]
X:	3.0	[px]	Y:	4.0
				[px]

Add boundary point

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

4.4 LC-Column:

Sample testSample
 Edit Display Settings

Gel 1D
add Gel 1D

Gel 2D
add Gel 2D

Lc Columns
add Lc Column

Other analyte 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 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.

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 “create/edit” page again.

Title:	test
--------	------

LC Column	Run Phases	Run Settings	Detection
Mobile phase components ?			
Mobile phase component:	myFirstComponent1	1.0	✗
Mobile phase component:	mySecondComponent2	2.0	✗
Add mobile phase component			
Gradient step 1: ?			
Gradient Type:	constant	12.0	[min]
Purpose:	aGoodPurpose	 ?	
Composition			
Component:	mySecondComponent2	2.0	✗
Add component			
Type:	calibration and washing	 ?	
Substance:	oneMoreTEstWithOneCompon	  ?	
Time	1.0	?	
Volume	2.0	? ✗	
Add between run			
Gradient step 2: ? ✗			
Gradient Type:	gradient	12.0	[min]
Purpose:	asdfasdf	 ?	
Composition			
Component:	mySecondComponent2	3.0	4.0 ✗
Component:	myFirstComponent1	12.0	14.0 ✗
Add component			
Add between run			
Add gradient step			

Update


add Fraction




Nr.	FractionId	StartPoint	EndPoint	ProteinAssay		
1	fasfafd	1.0	2.0	3.0		✗

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.

Edit Fraction

 Details for the start point	
Time of start of fraction of interest	

FractionId:	fasfafd	
StartPoint:	1.0	
EndPoint:	2.0	
ProteinAssay:	3.0	

Update

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:

Sample testSample

 Edit Display Settings

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Other analyte 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 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.

Chemical Treatment Processing Steps

Nr.	Digestion	Derivatisations		
1	trypsinDigestion			

add Chemical Treatment Processing Step


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

Show Chemicaltreatment

 Edit Display Settings

Digestion:	trypsinDigestion
Derivatisations:	

add Treated Analyte

Nr.	Description		
1	myTreatedSample		

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.

New Treatedanalyte

Description:	
--------------	--

Create

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:

Sample testSample

 Edit Display Settings

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 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.

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 the same “create/edit” page again.

Edit Otheranalyteps

 Edit Display Settings

Name:

add other analyte

Nr.	Name		
1	otherAnalyte		

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.

New Otheranalyte

Name:

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

Sample testSample

 Edit Display Settings

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Other analyte Processing Steps

add Other Analyte Processing Step

Chemical Treatment Processing Steps

add Chemical Treatment Processing Step

Massspec Experiments

add/remove 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.

Massspecexperiment

 Query  Edit Display Settings

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

	Name	Raw File
<input type="checkbox"/>	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
<input type="checkbox"/>	Phosphb_bsa_2hto1l	
<input type="checkbox"/>	Phosphb_bsa_5hto1l	
<input type="checkbox"/>	Phosphb_bsa_1hto5l	
<input type="checkbox"/>	Phosphb_bsa_1hto2l	
<input type="checkbox"/>	Phosphb_bsa_1hto1l	
<input type="checkbox"/>	Phosphb_bsa_10hto1l	
<input type="checkbox"/>	Phosphb_bsa_1hto10l	

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

[Return](#)

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.

Sample Generation
Sample Processing
▼ GelSubstance
Add GelSubstance
Find All GelSubstances
▶ Gelmatrix
▶ Buffer
▶ Detectionagent
▶ Reagent
Mass Spectrometry
MS-Analysis
Management

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

New GelSubstance

Gelsubstanceld:

Component 1

Name:

Concentration:

[mmol]

Component 2

Name:

Concentration:

[mmol]

Add a component

Create

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

GelSubstances per page: 15 [25] 50 100

6 GelSubstances found

Page 1 of 1

go to page go

Nr.	GelSubstanceId			
1	anotherSubstance			
2	myGelSubstance			
3	claudias			
4	tesdfsafasdfas			
5	sdfaf			
6	testGel2dSubstance			

GelSubstances per page: 15 [25] 50 100

6 GelSubstances found

Page 1 of 1

go to page go

4.9 Gel Matrix

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

Sample Generation
Sample Processing
▶ GelSubstance
▼ Gelmatrix
Add Gelmatrix
Find All Gelmatrices
▶ Buffer
▶ Detectionagent
▶ Reagent
Mass Spectrometry
MS-Analysis
Management

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

New Gelmatrix

GelmatrixId:						
DescriptiveName:	<input type="text"/>	<input type="radio"/>	?			
MatrixType:	<input type="text"/>	<input type="radio"/>	?			
X:	<input type="text"/>	Y:	<input type="text"/>	Z:	<input type="text"/>	?
Percentage acrylamide:	<input type="text"/>			?		
Acrylamide:bisacrylamide:	<input type="text"/>			?		
Gel Part				X		
Name:	<input type="text"/>	<input type="radio"/>	?			
X:	<input type="text"/>	Y:	<input type="text"/>	Z:	<input type="text"/>	?
Percentage acrylamide:	<input type="text"/>			?		
Acrylamide:bisacrylamide:	<input type="text"/>			?		
Gel Part				X		
Name:	<input type="text"/>	<input type="radio"/>	?			
X:	<input type="text"/>	Y:	<input type="text"/>	Z:	<input type="text"/>	?
Percentage acrylamide:	<input type="text"/>			?		
Acrylamide:bisacrylamide:	<input type="text"/>			?		
Add a component						

Create

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

Gelmatrixs per page: 15 [25] 50 100

4 Gelmatrixs found

| Page 1 of 1 |

go to page go

Nr.	GelmatrixId	DescriptiveName			
1	testGelMatrix3	slab gel			
2	myMatrix	IPG strip			
3	testGelMatrix2	IPG strip			
4	testGelMatrix	IPG strip			

Gelmatrixs per page: 15 [25] 50 100

4 Gelmatrixs found

| Page 1 of 1 |

go to page go




4.10 Buffer

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

Sample Generation
Sample Processing
▶ GelSubstance
▶ Gelmatrix
▼ Buffer
Add Buffer
Find All Buffers
▶ Detectionagent
▶ Reagent
Mass Spectrometry
MS-Analysis
Management

With the “Add Buffer” you can add buffers.

New Buffer

BufferId:	<input type="text"/>
Buffer Type:	<input type="text"/> 
Component 1	
Name:	<input type="text"/>
Concentration:	<input type="text"/> [mmol]
Component 2	
Name:	<input type="text"/>
Concentration:	<input type="text"/> [mmol]
Add a component	
<input type="button" value="Create"/>	

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

Buffer


















[Query](#)[Edit Display Settings](#)

6 Buffers found

| Page 1 of 1 |

Buffers per page: 15 [25] 50 100

go to page go

Nr.	BufferId			
1	letsTryOneMoreBuffer			
2	anotherBuffer			
3	testAdding			
4	testAddAdding			
5	testInterAdding			
6	testWithComponents			

Buffers per page: 15 [25] 50 100

6 Buffers found

| Page 1 of 1 |

go to page go

4.11 Detection agent

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

Sample Generation
Sample Processing
▶ GelSubstance
▶ Gelmatrix
▶ Buffer
▼ Detectionagent
Add Detectionagent
Find All Detectionagents
▶ Reagent
Mass Spectrometry
MS-Analysis
Management

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

New Detectionagent

Name:	<input type="text"/>	?
PurposeDescription:	<input type="text"/>	ⓘ
AgentManufacturer:	<input type="text"/>	ⓘ
AgentModel:	<input type="text"/>	
OriginDescription:	<input type="text"/>	
Volume:	<input type="text"/>	
Concentration:	<input type="text"/>	
Antibody 1:		
Specificity:	<input type="text"/>	ⓘ
Species:	<input type="text"/>	
Target:	<input type="text"/>	
Antibody 2:	✗	
Specificity:	<input type="text"/>	ⓘ
Species:	<input type="text"/>	
Target:	<input type="text"/>	

Add antibody

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

Detectionagents per page: 15 [25] 50 100

4 Detectionagents found

Page 1 of 1

go to page go

Nr.	Name			
1	myDetectAgent			
2	nullValues			
3	detectAgent			
4	anotherDetectAgent			

Detectionagents per page: 15 [25] 50 100

4 Detectionagents found

Page 1 of 1

go to page go

4.12 Reagent

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

Sample Generation
Sample Processing
▶ GelSubstance
▶ Gelmatrix
▶ Buffer
▶ Detectionagent
▼ Reagent
Add Reagent
Find All Reagents
Mass Spectrometry
MS-Analysis
Management

With the “Add Reagent” you can add reagents.

New Reagent

ReagentId:

Component 1 ✗

Name:

Concentration: [mmol]

Component 2 ✗

Name:

Concentration: [mmol]

Add a component

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

Reagent						Query	Edit Display Settings
4 Reagents found						Reagents per page: 15 [25] 50 100	
Page 1 of 1						go to page <input type="text"/> go	
Nr.	ReagentId	Components					
1	testInterdimAdding						
2	testReagent	comp1 1.0 mmol					
3	anotherReagent	1comp 1.0 mmol 2comp 2.0 mmol					
4	oneMoreTEstWithOneComponent	oneComponent 100.0 mmol					
4 Reagents found						Reagents per page: 15 [25] 50 100	
Page 1 of 1						go to page <input type="text"/> go	

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.

Sample Generation
Mass Spectrometry
▶ Ionsource
▶ Mzanalysis
▶ Detection
▼ Massspecmachine
Add Massspecmachine
Find All Massspecmachines
▶ Controlsoftware
MS-Analysis
Management

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

New Massspecmachine

Name:	<input type="text"/>
Manufacturer:	<input type="text"/> 
ModelName:	<input type="text"/>
ManufactureDate:	<input type="text"/> 
Ionsource:	<input type="text"/> 
Mzanalysis:	<input type="text"/> 
Detection:	<input type="text"/> 
TuneFile:	<input type="text"/>
MethodFile:	<input type="text"/>
SignificantCustomizations:	<div><div></div></div>



Details for MS 1 level 

Resolution m/z:	<input type="text"/>	[m/z]
Resolution limit method:	<input type="text"/> 	
EstimatedMassAccuracies:	<input type="text"/>	[ppm]

Add details for an MS-level

Create

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:

Massspecmachines per page: 15 [25] 50 100				
1 Massspecmachines found		Page 1 of 1		go to page <input type="text"/> go
Nr.	Name	ModelName		
1	myMassspecmachine	myModel		

5.2 Ionsource:

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

Sample Generation

Mass Spectrometry

▼ Ionsource

Add Ionsource

Find All Ionsources

► Mzanalysis

► Detection

► Massspecmachine

► Controlsoftware

MS-Analysis

Management

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

New Ionsource

Name: mylonsource

Type:

ESI

MALDI



other

Create

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:































Ionsource

 Query  Edit Display Settings

9 Ionsources found

Page 1 of 1

Ionsources per page: 15 [25] 50 100
go to page go

Nr.	Name	Type			
1	test	ESI			
2	testIt	ESI			
3	maIdIT	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

Ionsources per page: 15 [25] 50 100
go to page go

5.2.1 Electrospray:

New IonSource

Name:	myTestIonSource		
Type:	ESI		

Supply

SupplyType:	fed	
CycleTime MS1:		[ms]

Add Cycle Time

Solvent

SolventComposition:		
SolventFlowrate:		
SolventFlowrateUnits:		

Interface

InterfaceManufacturer:		
InterfaceName:		
InterfaceCatalognumber:		
InterfaceDescription:		

Sprayer

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

Acceleration and Dissociation

Accelerationvoltage 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 “Accleration and Dissociation” there exists a second link “Add Accelerationvoltage”, where you can enter the acceleration voltages for each MS-level.

5.2.2 MALDI:

New Ionsource

Name:	myTestIonSource		
Type:	MALDI		

Plate and Matrix			
PlateComposition:			
MatrixComposition:			
DepositionTechnique:			

Voltage Settings			
GridVoltage:		[V]	
Acclerationvoltage MS1:		[V]	✗

Add Accelerationvoltage

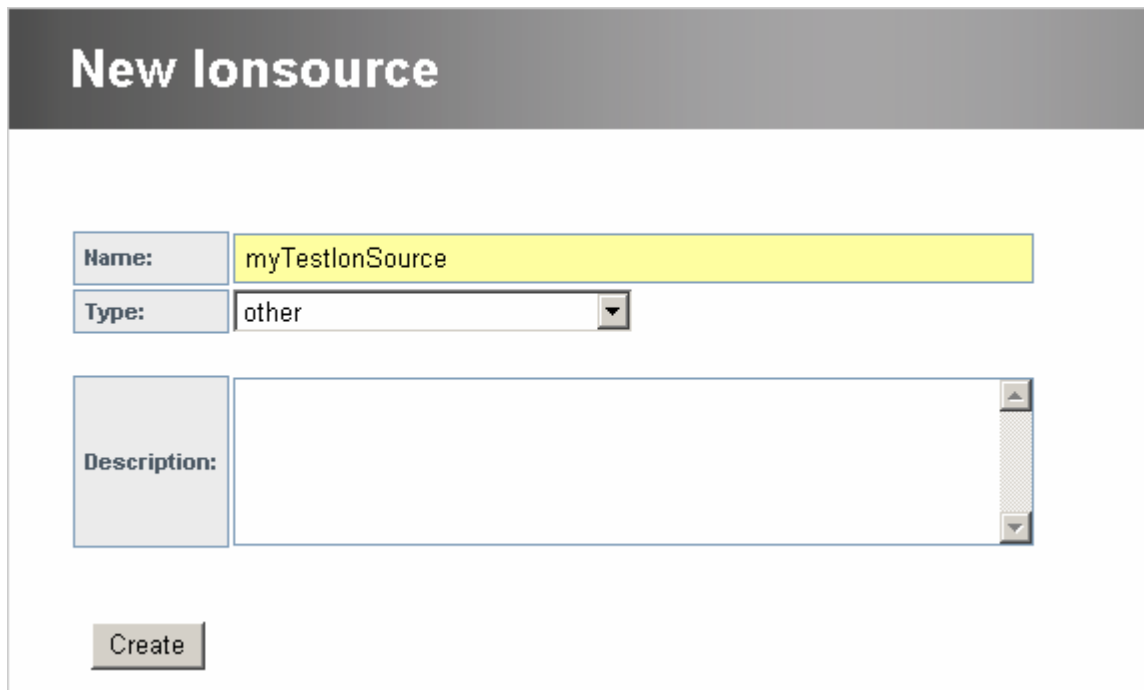
Post Source Decay			
PsdType:			
PsdDescription:			
ExtractionDelayed:	false		

Laser Settings			
LaserType:			
LaserWavelength:		[nm]	
LaserPower:		[microJ]	
FocusDiameter:		[microm]	
AttenuationDetails:			
PulseDuration:		[ns]	
ShotFrequency:		[Hz]	
AvgHrOfShotsFiredOnSpectrum:			

Create

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:



New IonSource

Name: myTestIonSource

Type: other

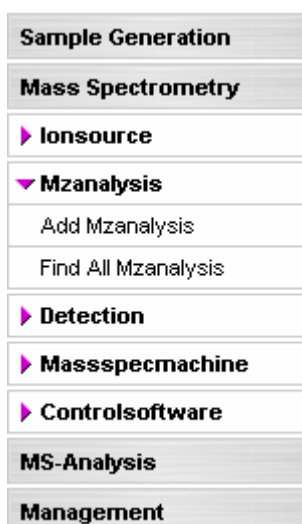
Description:

Create

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->Mzanalysis you reach the mzanalysis section.



- Sample Generation
- Mass Spectrometry
 - IonSource
 - Mzanalysis
 - Add Mzanalysis
 - Find All Mzanalysis
 - Detection
 - Massspecmachine
 - Controlsoftware
- MS-Analysis
- Management

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

New Mzanalysis

Name: myMzAnalysisApparatus

Type:

Create

- Ion Optic
- Quadrupole
- Hexapole
- TOF
- Ion Trap
- FT-ICR
- other

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

Query Edit Display Settings

Mzanalysis per page: 15 [25] 50 100

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

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

Mzanalysis per page: 15 [25] 50 100

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

5.3.1 Ion optic:

New Mzanalysis

Name:	myMzanalysisApparatus
Type:	Ion Optic
Description:	
Collisioncell:	<input type="checkbox"/>

Create

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:	<input type="checkbox"/>

Create

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:			<input checked="" type="radio"/>
GasPressure:		[bar]	
RfFrequency:		[Hz]	
ExcitationAmplitude:			
IsolationCentre:			
IsolationWidth:			
FinalMsLevel:			
Collisioncell:	<input type="checkbox"/>		

Create

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:	<div></div>		
Collisioncell:	<input checked="" type="checkbox"/>		
GasType:	<div></div>		
GasPressure:	<div></div>	[bar]	
CollisionOffset:	<div></div>		
CollisionEnergy:	<div></div>		

Create

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.

Sample Generation
Mass Spectrometry
▶ Ionsource
▶ Mzanalysis
▼ Detection
Add Detection
Find All Detections
▶ Massspecmachine
▶ Controlsoftware
MS-Analysis
Management

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

New Detection

Name:			
Type:	<input type="text"/>		
DetectorSensitivity:	<input type="text"/>		
RateOfDataAcquisition:	<input type="text"/>	<input type="text" value="[GHz]"/>	




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

Detection

 Query  Edit Display Settings

3 Detections found | Page 1 of 1 |

Detections per page: 15 [25] 50 100
go to page go

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

3 Detections found | Page 1 of 1 |

Detections per page: 15 [25] 50 100
go to page go

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.

Sample Generation
Mass Spectrometry
► Ionsource
► Mzanalysis
► Detection
► Massspecmachine
▼ Controlsoftware
Add Contr.Softws
Find All Contr.Softw.s
MS-Analysis
Management

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

New Controlsoftware

PackageName:	<input style="width: 80%;" type="text"/>
IsolationWidth:	<input style="width: 80%;" type="text"/>

Criteria

Criteria:
✗

Add Criteria

Softwares

Software:
▼
⊕
✗

Add Software

Create

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:

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.

Sample Generation
Mass Spectrometry
MS-Analysis
▼ Massspecexperiment
Add MS-Experiment
Find All MS-Experiments
Management

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

New Massspecexperiment

 Edit Display Settings

Name:	<input type="text"/>	
GenerationDate:	<input type="text"/>	
Massspecmachine:	<input type="text"/>	
Control and Analysis Software:	<input type="text"/>	
ParametersFile:	<input type="text"/>	
Raw File:	<input type="text"/>	
Description:	<input type="text"/>	

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:

File Upload

[Query](#)[Edit Display Settings](#)

Selected File: [Clean selection](#) [Accept Selection](#)

Files per page: [15](#) [\[25\]](#) [50](#) [100](#)

13 Files found

Page 1 of 1

go to page [go](#)

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

Files per page: [15](#) [\[25\]](#) [50](#) [100](#)

13 Files found

Page 1 of 1

go to page [go](#)

[Return](#)

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:

Massspecexperiments per page: **15** [25] 50 100

31 Massspecexperiments found

Page 1 of 2 | [Next >>](#)

go to page [go](#)





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

 Edit Display Settings

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

[Return](#)

[Update](#)

Added Searches

UploadName	PrepSteps
060606FTc2_phosphb_bsa_1hzu11	Sample: test
Mascot1hzu11	Sample: test
060606FTc2_phosphb_bsa_1hzu11Sequest	Sample: test
060606FTc2_phosphb_bsa_1hzu11SpectrMill	Sample: test
bsa_1hzu11XTandem	Sample: test

[add Massspec searches](#)

[Compare Results](#)

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.

File Upload

[Query](#) [Edit Display Settings](#)

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	<input type="text"/>		
SpectrumMill User Config File	<input type="text"/>		
XITandem Peptide Threshold:	30		
Omssa e-Value Threshold:	20		
Omssa Modification File	<input type="text"/>		
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

<input type="checkbox"/>	Upload Name	Category
<input type="checkbox"/>	11-15	spectrummill_old
<input type="checkbox"/>	060606FTc2_phosphb_bsa_2hzu1IXTandem	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

<input type="checkbox"/>	Upload Name	Category
<input type="checkbox"/>	060612_BSA_PhosphB_1heavyzu15light	mascot
<input type="checkbox"/>	060606FTc2_phosphb_bsa_2hzu1I	mascot
<input type="checkbox"/>	060606FTc2_phosphb_bsa_2hzu1IOMSSA	omssa
<input type="checkbox"/>	060606FTc2_phosphb_bsa_5hzu1I	mascot
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1ISequest	sequest
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1IXTandem	xtandem
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu5I	mascot
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu2IXTandem	xtandem
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu2I_A	mascot
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu2IOMSSA	omssa
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1I	mascot
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1IOMssa	omssa
<input type="checkbox"/>	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 if you have added modifications 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

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 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.

Searches

Query Edit Display Settings

Dbsearchparameterss per page: 15 [25] 50 100


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

Nr.	UploadName	PrepSteps	
<input type="checkbox"/>	SpectrumMill	Sample: forLexi,Spot: testSpectrMasc	
<input checked="" type="checkbox"/>	MascotCompSpectrMill	Sample: forLexi,Spot: testSpectrMasc	
<input checked="" type="checkbox"/>	SpectrumMill	Sample: forLexi,Spot: testSequMasc	
<input type="checkbox"/>	MSDB	Sample: forLexi,Spot: testSequMasc	

Dbsearchparameterss per page: 15 [25] 50 100

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

Accept

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:

Protein

[Query](#)
[Edit Display Settings](#)

1 = 060606FTc2_phosphb_bsa_1hzut11 (Partitioning [P](#))

2 = 060606FTc2_phosphb_bsa_1hzut10mssa (Partitioning [P](#))

3 = 060606FTc2_phosphb_bsa_1hzut10sequest (Partitioning [P](#))

4 = 060606FTc2_phosphb_bsa_1hzut10ctandem (Partitioning [P](#))

Proteins per page: [15](#) [25](#) [50](#) [100](#)

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	i
2	1 2 3 4	gi 162648	Bos taurus	albumin [Bos taurus]	42.81	30183.17	2	40	i
3	1 4	gi 435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	365.40	7	9	i
4	1 2 4	gi 136429		Trypsin precursor	68.3	237.20	3	6	i
5	4	gi 11967711	Homo sapiens	anaphase promoting complex subunit 1-Tsg24 protein [Homo sapiens]	5.92	154.00	1	4	i
6	4	gi 31560568	Mus musculus	NAD homolog 2 [Mus musculus]	7.29	95.30	1	3	i
7	4	gi 295721	Gallus gallus	conalbumin [Gallus gallus]	5.11	70.00	1	2	i
8	4	gi 124260		H3_0	20.0	73.30	5	2	i
9	4	gi 4865281	Homo sapiens	glutamate dehydrogenase 1 [Homo sapiens]	3.41	77.09	1	2	i
10	4	gi 124286		DegP (Arabidopsis thaliana)	8.46	70.20	1	2	i
11	4	gi 4509573		Structural maintenance of chromosome 1-like 1 protein (SMC1alpha protein) (SB1.8/CDV8423E protein) (SB1.8) - Homo sapiens (Human).	5.11	83.70	1	2	i
12	4	gi 27542557	Homo sapiens	EV22 protein variant [Homo sapiens]	2.06	68.59	2	2	i
13	4	gi 124319		MBP_Bora	3.97	45.90	1	1	i
14	4	gi 1083952		subtilisin-trypsin inhibitor, SIL13 - Streptomyces galbus [MASs=10982]	21.11	38.70	1	1	i
15	4	gi 124230		human pds5 (h.EST: Z42154 and fragment: K5A0648 plus HeLa N-term cDNA, see E. Vorlaender, Ph.D thesis 2002, pp. 49)	1.72	35.40	1	1	i
16	4	gi 8250019		beta-galactosidase [Cloning vector pBRINT-TsCm]	2.77	35.40	1	1	i
17	4	gi 6322830	Saccharomyces cerevisiae	Cdc16p [Saccharomyces cerevisiae]	1.43	44.80	1	1	i

Proteins per page: [15](#) [25](#) [50](#) [100](#)

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 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 [i](#) button you get all proteins of that cluster listed.

Protein

Query Edit Display Settings

- 1 = 060606FTc2_phosphb_bsa_1hzu1l (Partitioning)
- 2 = 060606FTc2_phosphb_bsa_1hzu1Omssa (Partitioning)
- 3 = 060606FTc2_phosphb_bsa_1hzu1Squest (Partitioning)
- 4 = 060606FTc2_phosphb_bsa_1hzu1KTandem (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	gil231300		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	gil162648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	2	40	
3	4	gil435476	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

Export Current View: Excel | DOC | TEXT

Details from

Nr.	Search	AccessionNum	Organism	GeneName	SequCovMax	Score	Cluster Nr.	Amount of Peptides
1	1 2 4	gil162648	Bos taurus	albumin [Bos taurus]	42.00988467874794	30183.173493681086	Cluster-3 Cluster-3 Cluster-7	40
2	1 2 3 4	gil418694	validated	serum albumin precursor [validated] - bovine	40.362438220757824	30102.723156271586	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40

To Protein View >>

To Peptide View >>

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.

Protein

Query Edit Display Settings

- 1 = 060606FTc2_phosphb_bsa_1hzu1l (Partitioning)
- 2 = 060606FTc2_phosphb_bsa_1hzu1Omssa (Partitioning)
- 3 = 060606FTc2_phosphb_bsa_1hzu1Squest (Partitioning)
- 4 = 060606FTc2_phosphb_bsa_1hzu1KTandem (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	gil231300		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	gil418694	validated	serum albumin precursor [validated] - bovine	40.37	30102.72	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
3	1 2 4	gil162648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
4	4	gil435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	355.40	Cluster-1	9
5	4	gil1346343		Keratin, type II cytoskeletal 1 (Cytokeratin 1) (CK1) (67 kDa cytokeratin) (Hair alpha protein)	13.2	337.19	Cluster-2 Cluster-2 Cluster-4 Cluster-1	8
6	4	gil39794653	Homo sapiens	Keratin 1 [Homo sapiens]	13.2	337.19	Cluster-2 Cluster-2 Cluster-1	8
7	4	gil71528		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

Export Current View: Excel | DOC | TEXT

<< To Cluster View

To Peptide View >>

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.

Export Current View: Excel | DOC | TEXT | PRIDE XML

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.

Concerning the querying:

The meaning of most of the query fields is clear by the name they carry. And most of the query fields are executed as directly on the database which is quite fast. The queries that are described here are post-database filters, that means that elements that do not meet the criteria are removed later, which takes a little bit longer:

























- **NrOfDifferentPepSequences:** a specific amount of peptide sequences (irrespective if they are carrying different modifications) must be found for one protein in one search
- **NrOfSpectraForPepSequence:** a specific amount of spectra must be found for one peptide sequence in one search (irrespective if they are carrying different modifications)
- **NrOfFhSpectraForPepSequence:** a specific amount of first hit spectra must be found for one peptide sequence in one search (irrespective if they are carrying different modifications)
- **NrOfDifferentPepSeqAndModi:** a specific amount of peptide sequences (each modified peptide is count as a separate peptide sequence) must be found for one protein in one search
- **NrOfSpectraForPepSequAndModi:** a specific amount of spectra must be found for one peptide sequence in one search (each modified peptide is count as a separate peptide sequence)
- **NrOfFhSpectraForPepSequAndModi:** a specific amount of first hit spectra must be found for one peptide sequence in one search (each modified peptide is count as a separate peptide sequence)
- **TotalSpectraForPepOfSearches:** a specific amount of spectra must be found for one peptide of a protein over several searches
- **TotalFhSpectraForPepOfSearches:** a specific amount of first hit spectra must be found for one peptide of a protein over several searches
- **SpectraForOneProteinFromMultiSearches:** a specific amount of spectra must be found for one protein over several searches
- **FhpectraForOneProteinFromMultiSearches:** : a specific amount of first hit spectra must be found for one protein over several searches

7.2 Cluster (Partitioning):

Partitioning



Clusters per page: [\[15\]](#) [25](#) [50](#) [100](#)

4 Clusters found
Page 1 of 1
go to page go

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						
3	Cluster-0003	albumin [Bos taurus]	2	30183.17	30142.95						
4	Cluster-0004	Glycogen Phosphorylase b (E.C.2.4. ...	1	51846.46	51846.46						


Clusters per page: [\[15\]](#) [25](#) [50](#) [100](#)


4 Clusters found
Page 1 of 1
go to page go


 Refresh
 Return



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

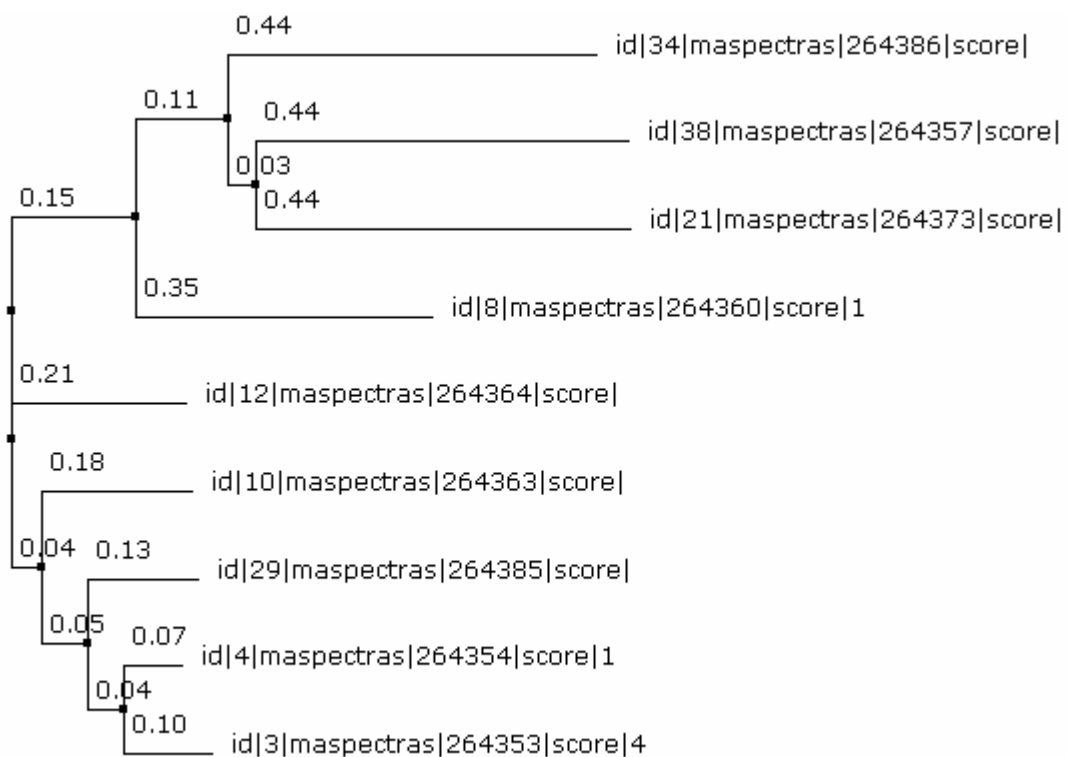
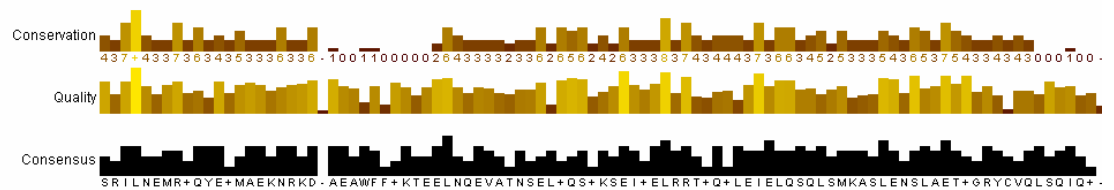
 : Download the storage of the tree that you can see in Jalview at the end of this section

 : The log-file of the alignment

 : 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

id|3|maspectras|264353|score|4|1-78: S R I L N E M R D Q Y E Q M A E K N R K D A E T W F L S K T E E L N K E V A S N S E L V Q S G R S E V T E L R R V L Q G L E I E L Q S Q L S M K A S L E N S L E E T K G R Y C M Q L S Q I Q G .
 id|4|maspectras|264354|score|1|1-78: S R I L N E M R D Q Y E K M A E K N R K D A E E W F F T K T E E L N R E V A T N S E L V Q S G K S E I S E L R R T M Q N L E I E L Q S Q L S M K A S L E N S L E E T K G R Y C M Q L S Q I Q E .
 id|29|maspectras|264385|score|1-78: S R I L N E M R D Q Y E K M A E K N R K D A E D W F F S K T E E L N R E V A T N S E L V Q S G K S E I S E L R R T M Q A L E I E L Q S Q L S M K A S L E N L A E T E N R Y C V Q L S Q I Q G .
 id|10|maspectras|264363|score|1-78: A K I L T D M R S D Y E A M V E K N R S D A E A W F T S K T D E L N Q E V A V H T K L L Q T S K T E V T D L R R T L Q G L E I E L Q S Q L S M K A L E G T L A E T E A R Y G V Q L S Q I Q A .
 id|12|maspectras|264364|score|1-78: Q L L N N M R S D Y E Q L A E Q N R K D A E A W F N E K S K E L T T E I D N N I E Q I S S Y K S E I T E L R R N V Q A L E I E L Q S Q L A L K Q S L E A S L A E T E G R Y C V Q L S Q I H A .
 id|8|maspectras|264360|score|1-78: D S I I A E V M A D Y E E I A N R S R T E A E S W Y Q T K Y E E L Q Q T A G R H G D L R N T K H E I S E M N R M I Q R L R A E I D N V K K Q C A N L N A I A D A E Q G E L A L K D A R N .
 id|34|maspectras|264386|score|1-78: P A I I S S S N S N K N E N A V S T D T S T P A A A G A P E G K P P Q K T S N K K S L S S K E A I E E L K H F S E K F K V P Y D I P K D M L E V L K R S S T L K S N S L P P K P I S K I .
 id|21|maspectras|264373|score|1-78: S V L L R L A E Y E A T L E E C C A K D D P H A C Y S T V F D K L K H L V D P Q N L I K Q N C D Q F E K L G E Y G F Q N A L I V R Y T R K V P Q V S T P T L V E V S R S L G K V G T R C T I .
 id|38|maspectras|264357|score|1-78: L G I K G K N L Y L S C V M K D N T P T L Q L E D I D P K R Y E K R D M E K R F V F Y T E I K N R V E F E A L Y P N W Y I S T S Q A E Q K R V F L G N



7.3 Peptide comparison:

ABBOS serum albumin precursor [validated] - bovine

Query
 Edit Display Settings
 Show Sequence

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

Sequence

```
MKWVTFISLLLLFSSAYS SRGVFRDRTHKSEIAHRFKDLGEEQFKGLVLIAFSQYLQQCPFDEHVKLVNE
LTEFAKTCVADESHAGCEKSLHTLFGDELCKVASLRETYGDMADCCEKQEPERNECFLSHKDDSPDLPKL
KPDPNTLCDEFKADEKKFWGKYLYEIAARRHPYFYAPELLYYANKYNGVFQDCQAEDKGACLLPKIETMR
EKVLASSARQRLRCASIQKFGERALKAWSVARLSQKFPKAEFVEVTKLVTDLTKVHKECCHGDLLECADD
RADLAKYICDNQDTISSKLKECCDKPLLEKSHCIAEVEKDAIPENLPPLTADFAEDKDVCKNYQEAKDAF
LGSFLYEYSRRRHPEYAVSVLLRLAKEYEATLEECCAKDDPHACYSTVFDKLKHLVDEPQNLIKQNCDFE
KLGEYGFNALIVRYTRKVPQVSTPTLVEVSRLGKVGTRCTKPESERMPCTEDYLSILNRLCVLHEK
TPVSEKVTKCCTESLVNRRPCFSALTPDETYPVKAFDEKLFTFHADICTLPDTEKQIKKQTALVELLKHK
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

[Compare Ratios of 2 Modifications](#)

105 Peptidehits found
Page 1 of 5 | [Next >>](#)
go to page [go](#)

	Search	Score	Sequence	
<input checked="" type="checkbox"/>	3	91.35	.M%PCTE@D@YLSILNR.@	i
<input checked="" type="checkbox"/>	3	75.42	.MPCTE@D@YLSILNR.@	i
<input checked="" type="checkbox"/>	1 2 3	71.02	.LGE@YGFQNALIVR.@	i
<input checked="" type="checkbox"/>	1 2 3	70.71	.LGE*YGFQNALIVR.*	i


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. At the upper right part of the peptides listed there is the link “Compare Ratios of 2 Modifications”. Here you can compare the quantitative ratios of differentially

labelled proteins (e.g ICPL-light to ICPL-heavy), or all found peptides which carry a modification versus ones that do not carry the modification (see 7.6).

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	
<input checked="" type="checkbox"/>	1	45.59	.TVM%E*NFVAFVD*K.*		
<input checked="" type="checkbox"/>	1	63.65	.TVM%E@NFVAFVD@K.@		
<input checked="" type="checkbox"/>	1	34.19	.VPQVSTPTLVE@VSR.@		
<input checked="" type="checkbox"/>	1	49.59	.VPQVSTPTLVE*VSR.*		
<input checked="" type="checkbox"/>	1	24.34	.YICD@NQD@TISSK.@		
<input checked="" type="checkbox"/>	1	45.04	.YICD*NQD*TISSK.*		
<input checked="" type="checkbox"/>	1	26.62	.YICDNQD@TISSK.@		
<input checked="" type="checkbox"/>	1	34.54	.YLYE*IAR.*		
<input checked="" type="checkbox"/>	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	Numlons	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	Numlons	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.

Details from SGSLTFNSK							X
Nr.	Search	Score	Sequence	Mass	Delta	NumIons	ParentCharge
1	2	48.03	.SGSLTFNSK.	940.473935	0.777138	7	2
2	2	42.94	Franz2.0735.07372.dta	73935	2.117138	6	2
3	1	15.82	51.25 .SGSISYLGR.	74	0.7582		2
4	1	13.8	48.03 .SGSLTFNSK.	.SGSLTFNSK.	940.474	2.1182	2

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).

When you click on the link on the peak area entries you receive a chromatogram viewer for the manual inspection and correction of the automatically calculated peak areas (see 7.5.)

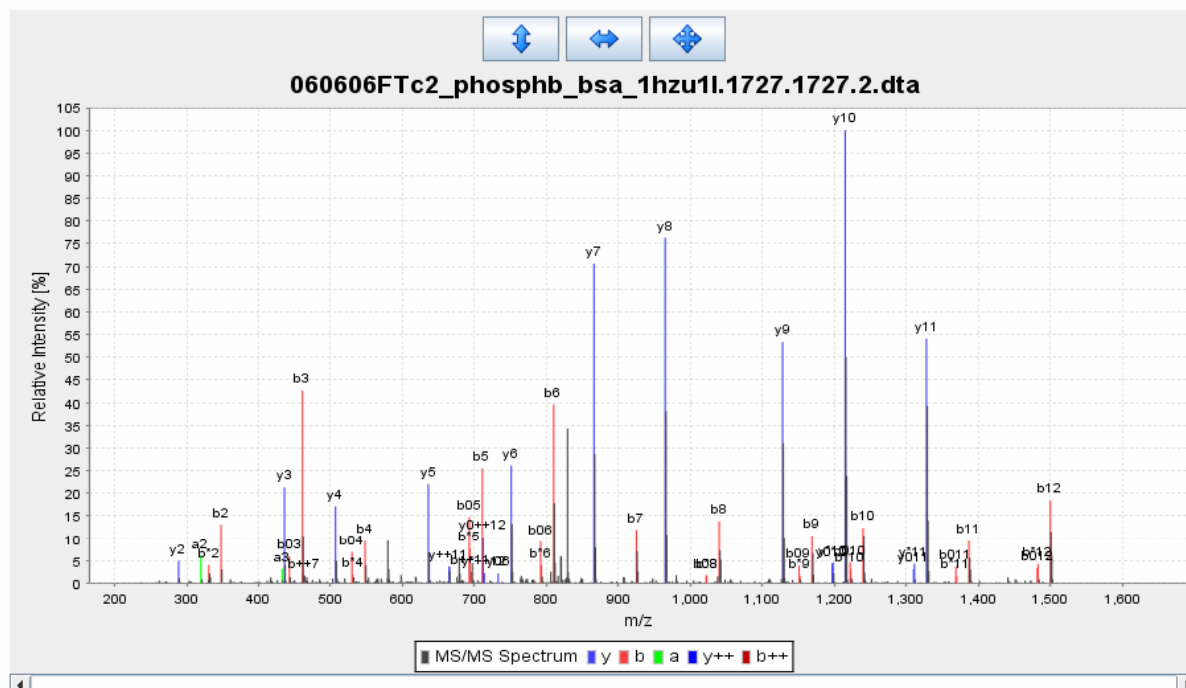
Concerning the querying:

The meaning of most of the query fields is clear by the name they carry. And most of the query fields are executed as directly on the database which is quite fast. The queries that are described here are post-database filters, that means that elements that do not meet the criteria are removed later, which takes a little bit longer:

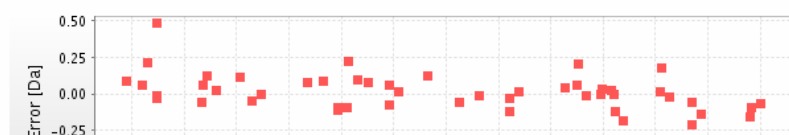
- **NrOfPassingSpectra:** a specific amount of spectra must be found for one peptide hit in one search
- **NrOfPassingFirstHitSpectra:** a specific amount of spectra must be found for one peptide hit in one search
- **NrOfTotalPassingSpectra:** a specific amount of spectra must be found for one peptide hit in several searches
- **NrOfTotalPassingFirstHitSpectra:** a specific amount of spectra must be found for one peptide hit in several searches

7.4 Spectrum View:

K@LLSYVDDEAFIR



	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	

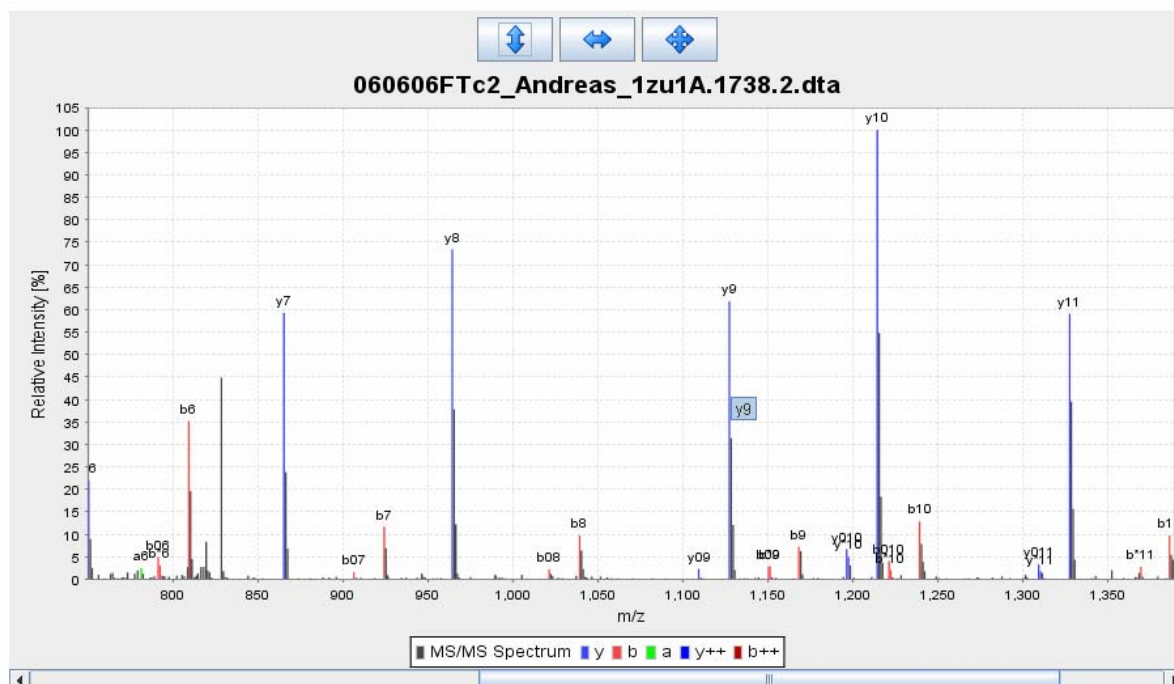


With “Edit Display Settings” you can select the series you want to be displayed. You can save your own display settings like in all the other pages.

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

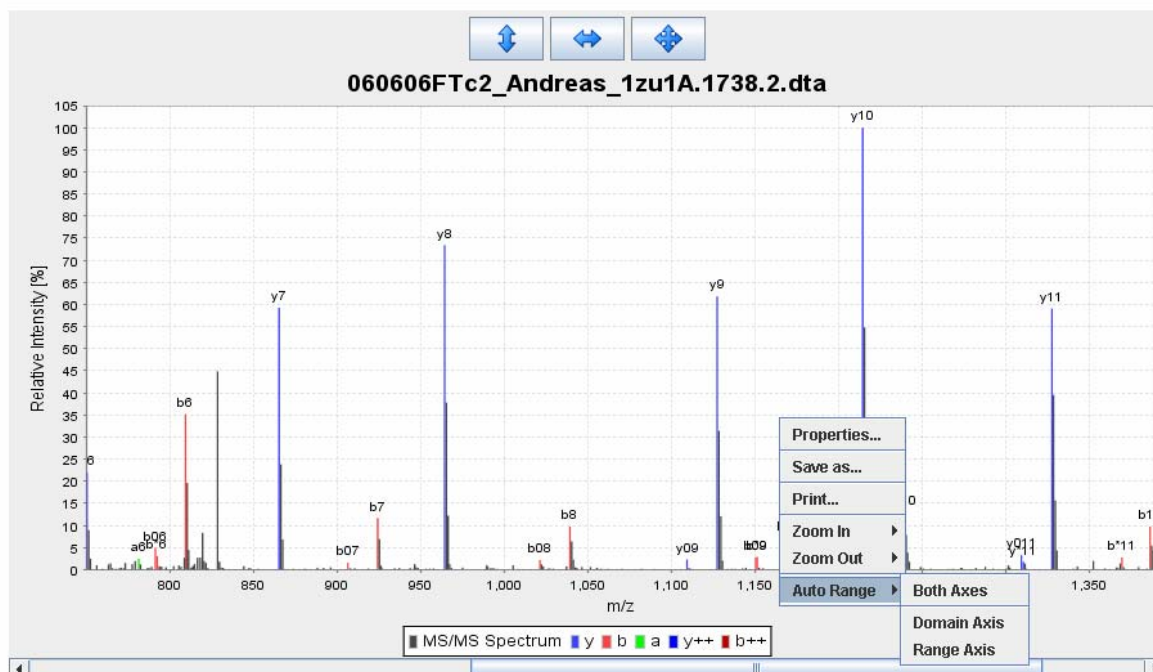


: zooms out the x-axis

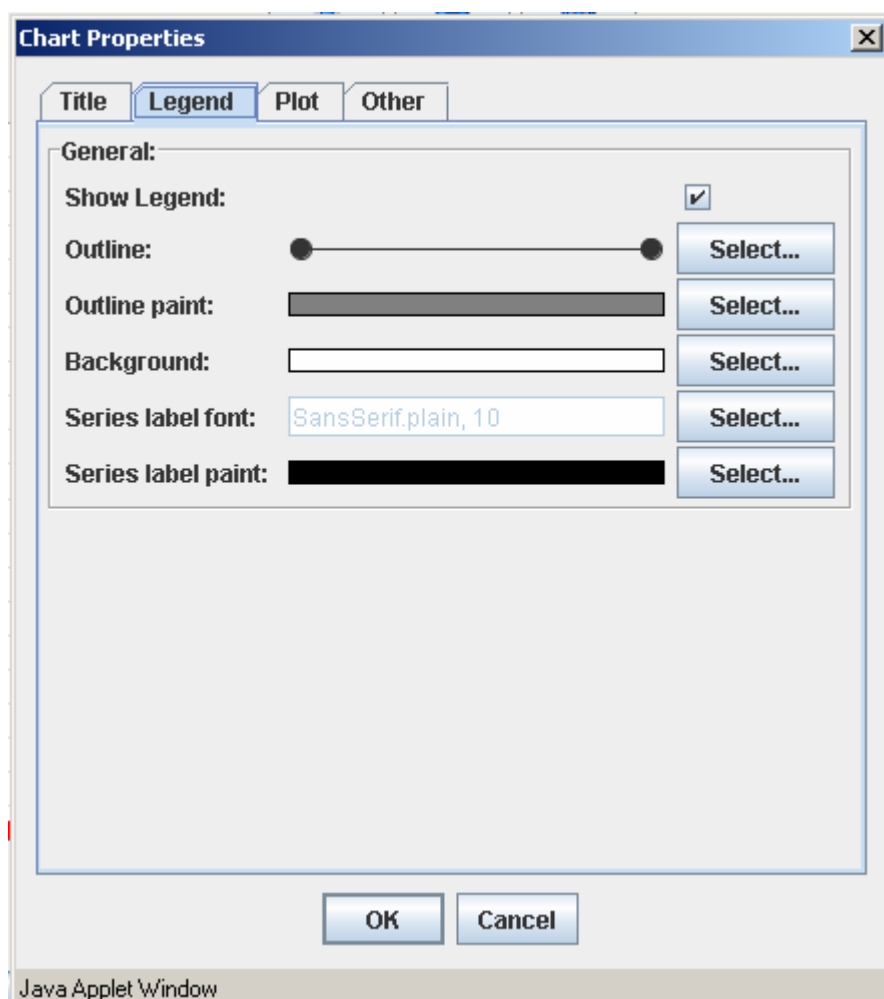


: zooms out both axes

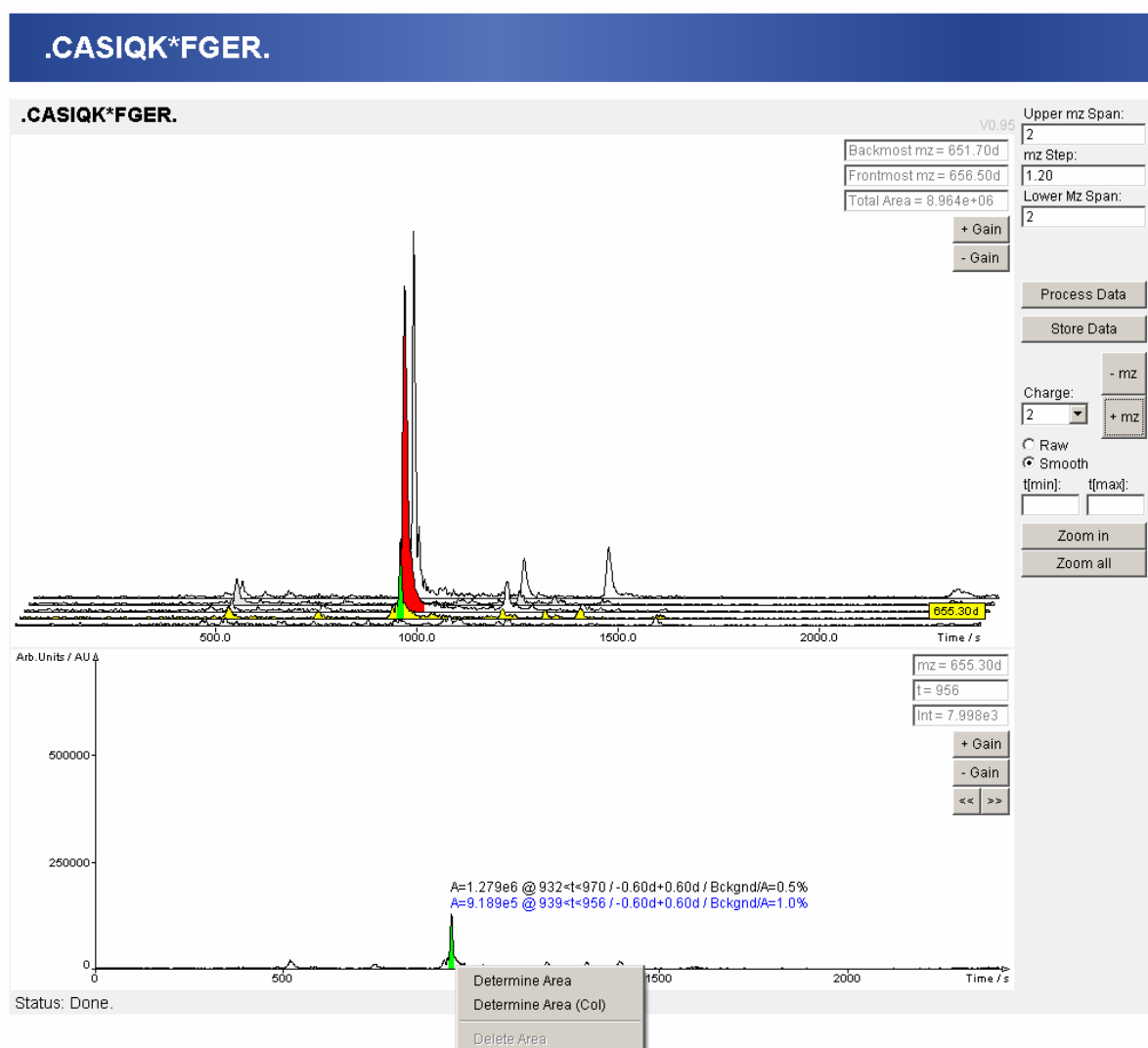
When you first click on the spectrum and then click with the right mouse button you will get a popup window where you have additional features:



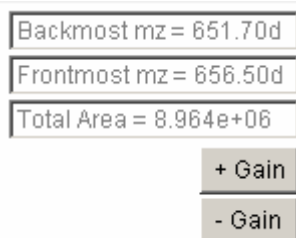
You can print your actual zoom scan. In the “Properties...” you can customize your font and other settings.



7.5 Chromatogram viewer



At the top the name of the peptide is written. The upper view shows the chromatogram plus the chromatograms in the neighbourhood. The red peak is the quantified one the green peak indicates one that has been selected manually. The second view shows one of the upper chromatograms in a 2 dimensional view. The one chromatogram which has been selected is shown in yellow in the upper view. The mass to charge ratio of the selected chromatogram is shown in the yellow box on the right side of the upper view.



The box at the upper right part of the upper view shows the m/z borders where the chromatograms are depicted and the total area calculated. With “+Gain” and “-Gain” you can zoom in and out the amplitude.

Upper mz Span:

 mz Step:

 Lower Mz Span:

Process Data

Store Data

Charge:

☐ Raw
☒ Smooth

t[min]:
 t[max]:

Zoom in

Zoom all

In the menu on the right side you can determine how many chromatograms you want to see in positive/negative m/z direction with “Upper mz Span”/”Lower Mz Span”. With the mz Step you can select the distance between two chromatograms. Peaks within one half of the distance in positive direction and one half of the distance in negative direction are taken for the calculation of the chromatograms. Once you changed something there you must press the “Process Data” button to retrieve the chromatograms from the server. The “Store Data” button stores manually changes (additional or removed peaks). With the “Charge” you can switch between the charge states of the peptide (only found charge states are calculated). With the “-mz” and the “+mz” you can select the chromatogram for the 2D view. With “Raw” and “Smooth” you can see the smoothed chromatogram and the raw chromatogram. In the “t[min]” and “t[max]” you can fill in the time borders and with “Zoom in” you can zoom to this borders for the 2D view. Use “Zoom all” to go back.

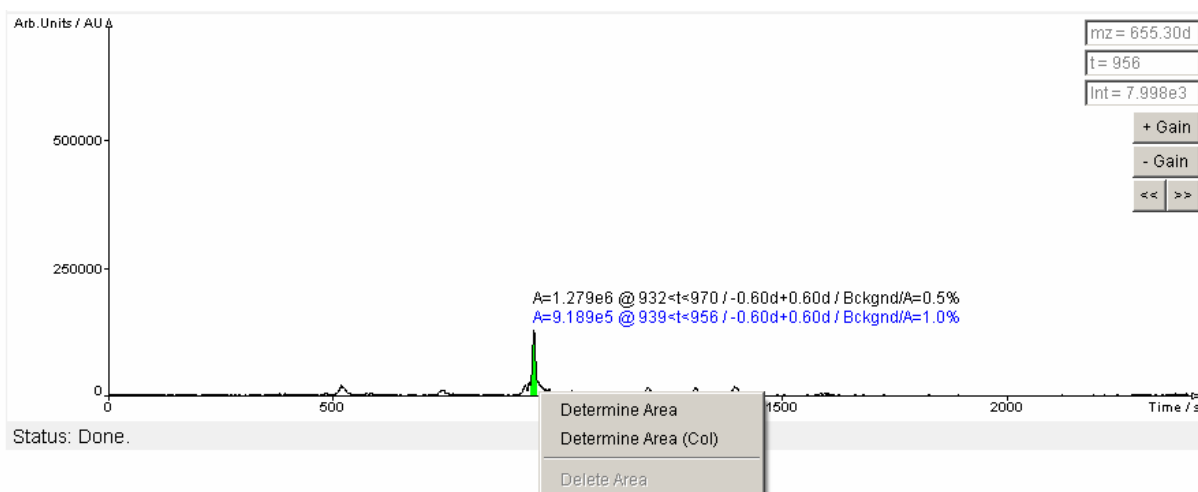
mz = 655.30d
 t = 956
 Int = 7.998e3

+ Gain

- Gain

<< >>

The box at the upper right part of the lower view shows the current m/z value, the time where the cursor is actually and the amplitude where the cursor is actually. With “+Gain” and “-Gain” you can zoom in and out. With “<<” “>>” you can move in the zoomed view left and right.

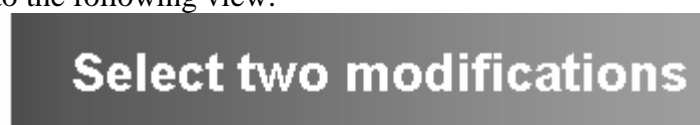


In the lower view you can select and deselect peak areas when you move the cursor inside the peak area you want to select and click the right mouse button the popup will appear. With the “Determine Area” you select a peak like it is chosen in ASAPRatio. With “Determine Area

(Col)” the new peak finding algorithm is taken which quantifies peaks with saddle-points and foothills. The black “A=...” shows the stored area in the database the blue “A=...” shows the actually selected area for that peak. If a peak with the same boundaries is stored in the database the peak appears in red otherwise it is shown in green. At the bottom there is a progress bar. When there “Done” appears you can work on the chromatograms, when “Processing Data ... “ the applet is fetching data from the server and there is no use to work on the data now because the data will be overwritten when it is finished.

7.6. Evaluation of quantitative ratios

When you click on the link “Compare Ratios of 2 modifications” in the peptide list you come to the following view:



	Search
<input type="checkbox"/>	N-termXK*: 111.04
<input type="checkbox"/>	N-termXK@: 105.02
<input type="checkbox"/>	XM%: 15.99

Accept

Here all the possible variable modifications are listed. You can select one or two between them you want to calculate ratios and click the “Accept” button.

(See next figure) At the upper left the selected searches are listed and a number for them. Then you have a list of your comparable peptides. In the first column you can select and deselect the peptide, the second column indicates the search which is compared, the third column is the peptide sequence which is compared, the fourth column shows the charge states which are comparable, the fifth column shows the area for one modification, the sixth for the other one, the seventh and the eighth column shows the ratios of the areas to one another. At the end of the column the mean and the standard deviation of the selected values is calculated. The whole list can be exported to Excel, Doc and txt. At the bottom of this is a link called “Refresh areas” which refreshes the list when you changed quantified areas manually. The picture depicts the found ratios graphically and calculates a regression line for the values. On the one axis the area for one modification and on the other to area for the other modification is depicted. The picture can be copied directly out of the browser.

1=ICPL_Protmix_1Iizu1he_A_c1_ms2
2=ICPL_Protmix_1Iizu1he_B_c1_ms2
3=ICPL_Protmix_1Iizu1he_C_c1_ms2

	Sequence	Z	N-termXK*: 111.04	N-termXK@: 105.02	Ratio 1/2	Ratio 2/1	
<input checked="" type="checkbox"/>	3	.ALK*AWSVAR.	2	8856610.6171875	8761861.0	1.0108138690156692	0.9893018197047497
<input checked="" type="checkbox"/>	2	.ALK*AWSVAR.	2	9542612.75	9225358.75	1.0343893401435473	0.9667539689274303
<input checked="" type="checkbox"/>	1	.ALK*AWSVAR.	2	1.0170150546875E7	9550851.375	1.0648423001844691	0.9391061942475086
<input checked="" type="checkbox"/>	2	.CASIQK*FGER.	3	876386.25	958544.125	0.9142888961945284	1.0937461935305353
<input checked="" type="checkbox"/>	1	.CASIQK*FGER.	2	9323722.59375	9311852.25	1.0012747564535294	0.9987268664816393
<input type="checkbox"/>	3	.CLK*DGAGDVAQVK.	2	128293.22	661789.1	0.19385816417949464	5.15841055357407
<input type="checkbox"/>	2	.CLK*DGAGDVAQVK.	2	195198.17	634894.9	0.30744957945007906	3.2525658411654166
<input type="checkbox"/>	3	.CLVEK*GDVAQVK.		0.0	0.0	NaN	NaN
<input checked="" type="checkbox"/>	2	.CLVEK*GDVAQVK.	2	1307267.75	1664997.8046875	0.7851468310166081	1.2736471198708146
<input checked="" type="checkbox"/>	1	.CLVEK*GDVAQVK.	2	1319871.453125	1459752.2	0.9041750052680174	1.1059805835968424
<input checked="" type="checkbox"/>	3	.DDTVCLAK*LHDR.	2	2808382.15625	2191846.390625	1.2812860281915999	0.7804658585182535
<input checked="" type="checkbox"/>	3	.DHMK*SVIPSDGPSVACVK.	2	164365.38	166958.88	0.9844662350394301	1.0157788702219408
<div>⋮</div>							
<input checked="" type="checkbox"/>	1	.YLGEELYK*AVGNLR.	3	506337.73046875	416672.78125	1.2151927201718316	0.8229147388725283
		Mean:				0.9666037807938672	1.0660752058942036
		Standard Dev.:				0.16904034	0.18760616

Export Current View: Excel | DOC | TEXT

fresh Areas

