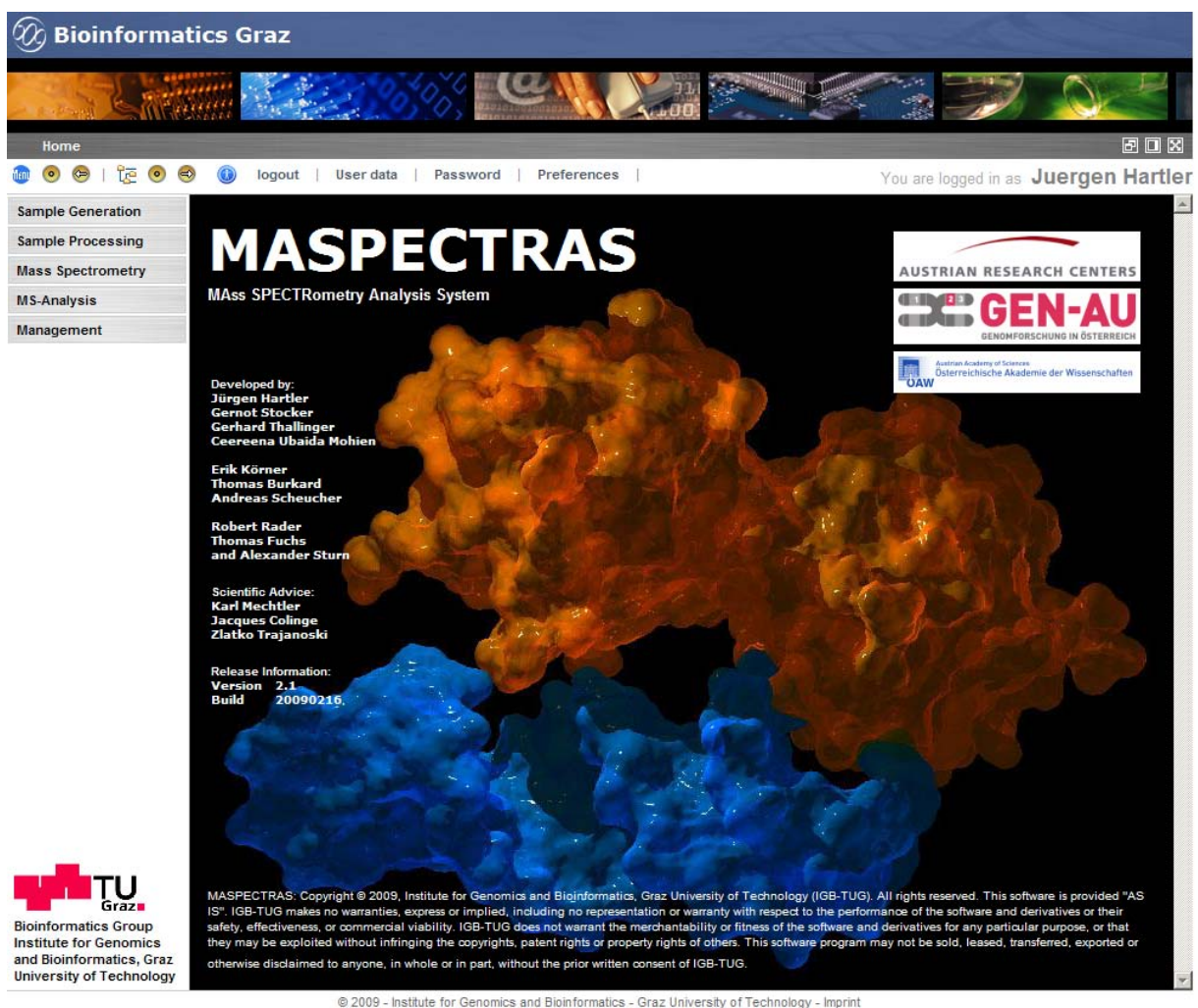


# MASPECTRAS

## Users Guide

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

### 1. General Information:



This will be your first impression of MASPECTRAS.

The main view is divided into 3 sections:

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

## 1.1 The header section:





### 1.1.1 The display bar:




The “Home”-link leads you back to the start page.

At the right side there are 3 icons where you can change the spatial usage of the browser window:



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


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

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

### 1.1.2 The menu administration bar:



This bar allows the customization of the menu bars. The icons which come after  change the settings of the normal menu while the icons which come after  change the settings of the tree menu. The meaning of the symbols is the same:

-  : this removes the menu bar on the left side of the screen so that all of the space is available for the main information page:

## Welcome to MASPECTRAS







**User name:** hartler  
**Full name:** Juergen Hartler  
**Email address:** juergen.hartler@tugraz.at  
**Institute name:** Bioinformatics Group  
**Valid since:** Sat Oct 09 12:28:37 CEST 2004  
**Valid until:** Thu Dec 31 12:28:37 CET 2009  
**Last login date:** 14.48.40:14.02.2008  
**Last login realm:** maspectras  
**Password expires:** never  
**Server Name:** localhost  
**Server Port:** 8080  
**Scheme:** http  
**Secure:** false









## Header Elements

**accept** image/gif, image/x-xbitmap, image/jpeg, image/pjpeg, application/x-powerpoint, application/msword, \*/\*

- : this shows a menu bar again on the left side (here the tree menu is shown):







[logout](#) | [User data](#) | [Password](#) | [Preferences](#)

Experiments

anotherSubNode


test ShowInTree

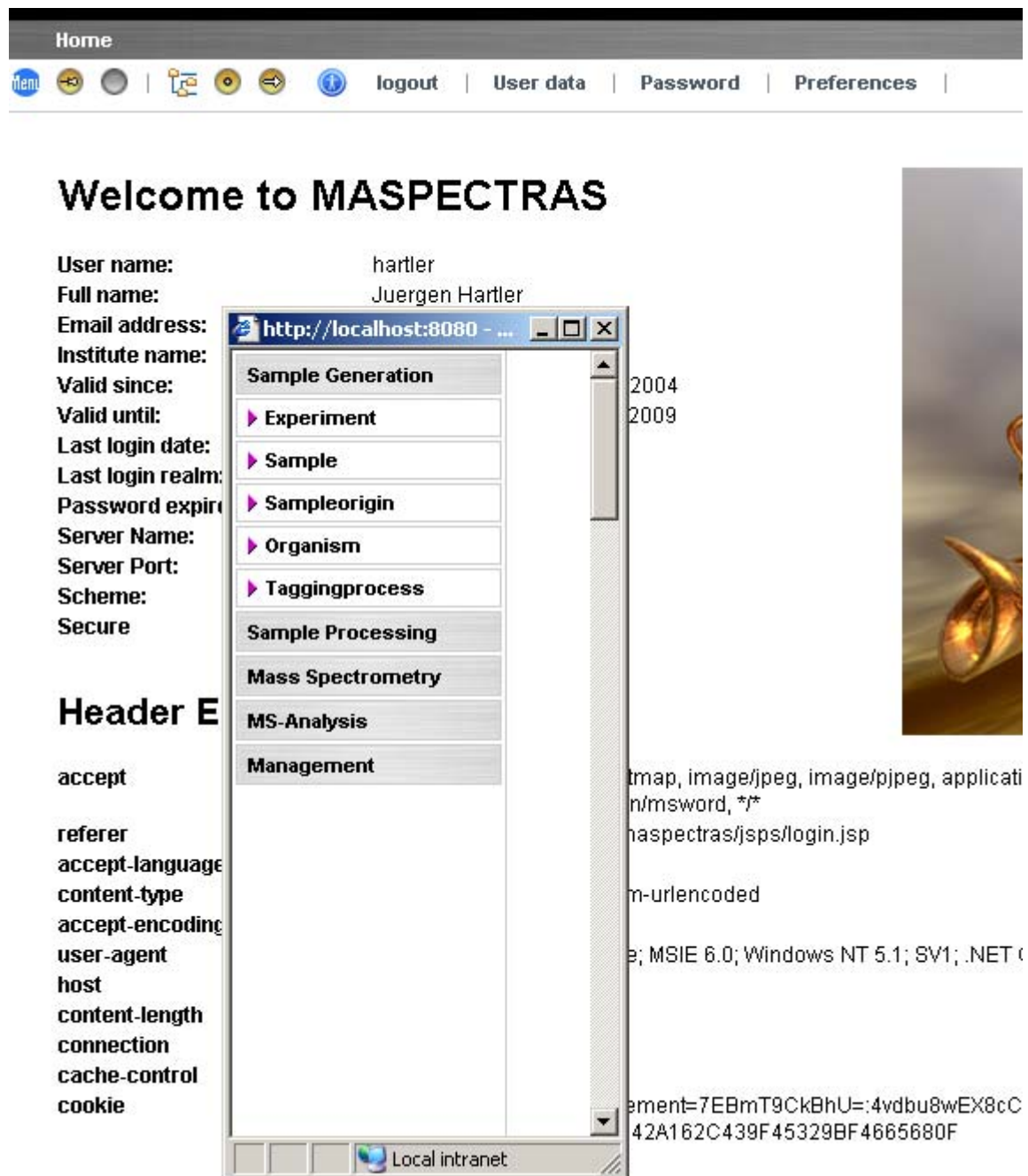
## Welcome to MASPECTRAS


**User name:** hartler  
**Full name:** Juergen Hartler  
**Email address:** juergen.hartler@tugraz.at  
**Institute name:** Bioinformatics Group  
**Valid since:** Sat Oct 09 12:28:37 CEST 2004  
**Valid until:** Thu Dec 31 12:28:37 CET 2009  
**Last login date:** 14.48.40:14.02.2008  
**Last login realm:** maspectras  
**Password expires:** never  
**Server Name:** localhost  
**Server Port:** 8080  
**Scheme:** http  
**Secure:** false

## Header Elements

**accept** image/gif, image/x-xbitmap, image/

: this shows a menu bar in a new window:



: this removes the opened window.

### 1.1.3 The user (login) bar:

If you are not logged in:

 login |

please login

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
- Sets the preferences for the display

### 1.1.3.1 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 (!"@"=?...).

### 1.1.3.2 Change Preferences:

Window Setup:	<input type="text" value="small-window"/>
Menu Setting:	<input type="text" value="left-side-menu"/>
Tree Setting:	<input type="text" value="not displayed"/>
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Bioinformatics Group"/>

This allows customization of the menu structure for each user. Whenever the user logs in the preferences are loaded and the menu display changes correspondingly.

Window-setup:

- small-window: same meaning like  in 1.1.1
- stretched-window: same meaning like  in 1.1.1
- fullscreen-window: same meaning like  in 1.1.1



The “Menu Setting” and the “Tree Setting” have the same options. The option “left-side-menu” is just possible for one of them, since otherwise too much space for the display of information is lost:


- left-side-window: the menu is displayed at the left side of the information screen (default setting for the “Menu Setting”)
- new-window-menu: the menu is displayed in a new window; for this option the pop-ups for the Maspectras application must not be blocked.
- not-displayed: the menu is displayed not at all.

The “Owned by” fields allow the specification of the default displayed ownership of entered or edited data. This is just for the default view, while in every page the change of the ownership is possible.

## 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 iheyensis 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				X
Masc/+1 Score	>	20		X
Masc/+2 Score	>	25		X
Masc/+3 Score	>	30		X
SMill/+1 Score	>	15		X
SMill/+2 Score	>	18		X
SMill/+3 Score	>	22	AND	X

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
<b>Required Information</b>		
<input checked="" type="checkbox"/> AccessionNum	<input type="checkbox"/> Organism	<input type="checkbox"/> Sequence
<input checked="" type="checkbox"/> GeneName	<input type="checkbox"/> OrfNumber	<input type="checkbox"/> Modifications
<input type="checkbox"/> Synonyms	<input type="checkbox"/> Description	<input type="checkbox"/> PredictedMass
	<input type="checkbox"/> PredictedPi	<input type="checkbox"/> Score
	<input type="checkbox"/> Nr. of Proteins	<input type="checkbox"/> Cluster Nr.
		<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	karIDB	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: **quantTestJune2006**

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

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

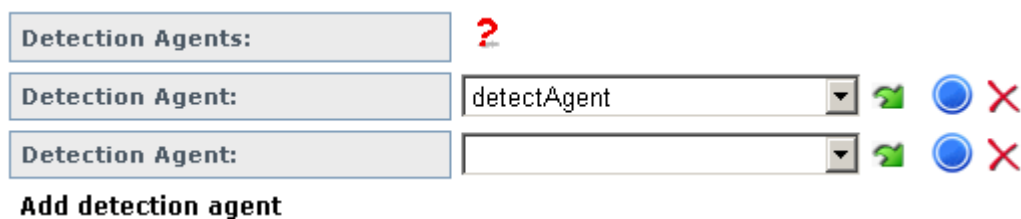
When you select a user or an institute the checkboxes at  and  are enabled and you can additionally specify if the user has edit or delete rights on your data.


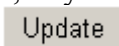

#### 1.2.4 Select input Fields:



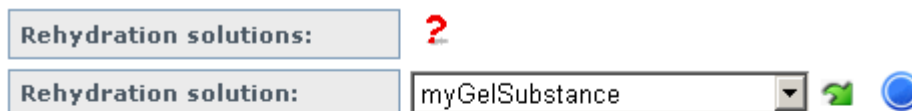
When you have an input field like the one above and your element of choice is not in the drop down menu, you can push the blue button and enter your element. The button can lead either to an input page of an element or to add dictionary elements. Dictionary elements are unified text elements. The main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

#### 1.2.5 Multiple input Fields and other buttons:






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

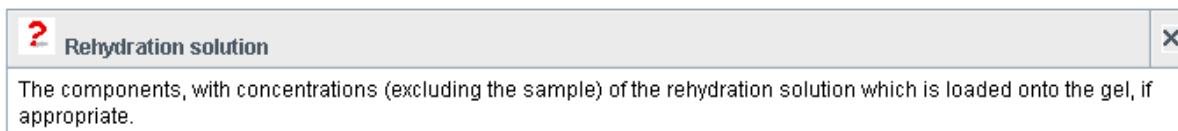
When you press the  Button you retrieve additional information about the selected object.



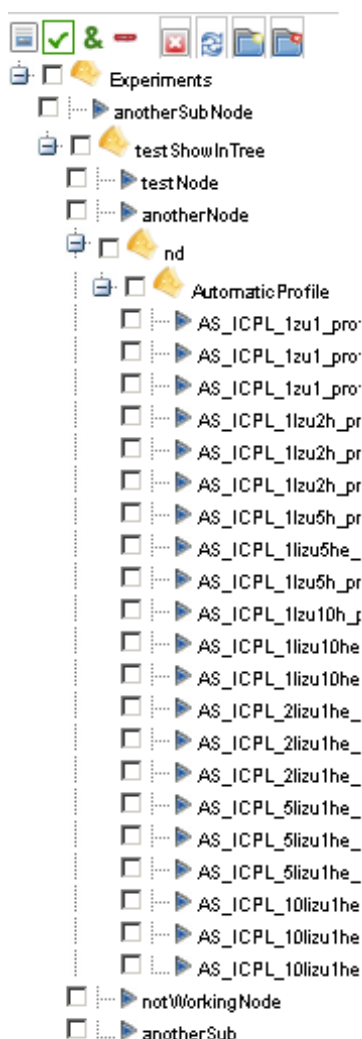
Details for gel matrix			
Component	Concentration		
componentOne	1.0		
componentTwo	2.0		

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.



### 1.3 The tree menu:



The tree menu has at the top the command line and below it is showing a tree existing of experiments and sub-experiments (see 3.1). Their child nodes can be samples (3.2) and the child nodes of the samples can be massspecexperiments (see 6.1).

In the top menu you have 3 different selection possibilities:

: shows all of the elements of this search and does not affect any of the other searches.

: shows all of the elements of this search and from the other elements just the ones which are in this search (just the common ones of several searches are shown)

: elements marked with this icon are subtracted from the rest of the selection.

For the selection of elements first the corresponding element has to be selected from the command line at the top, and then you have to click on the checkbox which you want to select.

To accept the selection click on

In the next picture you can see a selection. You can see that for the "&" and the "-" selection automatically queries has been generated. For the "&" the operator is "=" and for the "-" the operator is "<".


**Protein** Query Edit Display Settings


Query


UPLOAD NAME = AS\_ICPL\_1zu1\_profilesca ✖

UPLOAD NAME <> AS\_ICPL\_1zu1\_profilesca AND ✖

**Submit Query** | **Reset Query** | **Restore Default** Save Queries

1 = AS\_ICPL\_1zu1\_profilescan\_B\_c2.dat (Partitioning )

2 = AS\_ICPL\_1zu1\_profilescan\_C\_c2.dat (Partitioning )

3 = AS\_ICPL\_1zu1\_profilescan\_A\_c2 (Partitioning )

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

2 Proteins found | Page 1 of 1

Nr.	Search	AccNr	Organism	GeneName	%SeqMax	Score	# Prots	# Peps
1	2	gi 124408		ClpC	0.87	20.03	1	1
2	2	gi 124316		Wendt Kleisin Beta	4.74	20.43	1	1


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

2 Proteins found | Page 1 of 1

**Export Current View:** [Excel](#) | [DOC](#) | [TEXT](#) | [PRIDE XML](#)

[To Protein View >>](#)

[To Peptide View >>](#)

When a folder is selected the same operator is applied to all massspecexperiments which are in this folder. When a name of a folder or massspecexperiment is clicked for all of the massspecexperiments associated the  operation is applied.

Other menu items:



: unselects all of the selections





: refreshes the tree



: adds a new subexperiment to an experiment (will not work for samples or msexperiments)

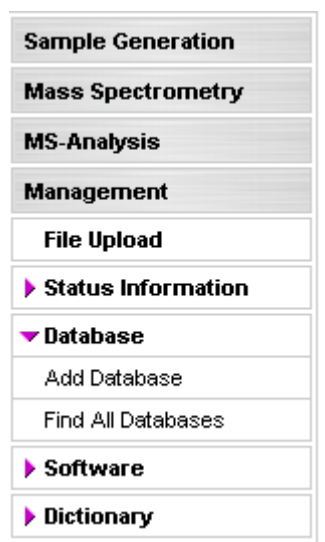


: moves one node to another one; the node to move must be marked with  and the receiving node with 

## 2. Management Section:

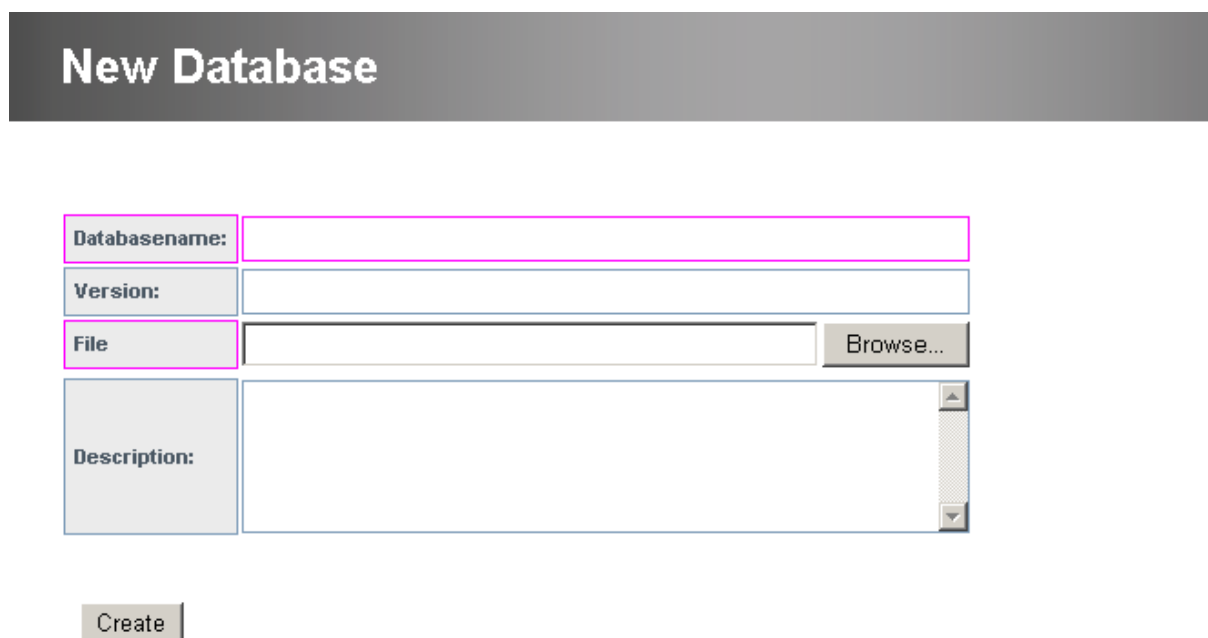
### 2.1 Database:

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.



A vertical menu titled 'Management' with several options. The options are: 'Sample Generation', 'Mass Spectrometry', 'MS-Analysis', 'Management' (highlighted), 'File Upload', '► Status Information', '▼ Database' (expanded), 'Add Database', 'Find All Databases', '► Software', and '► Dictionary'.

With the “Add Database” you can add a new database. The second possibility to upload a database is the MultipleFiluploadApplet (see 2.2). This applet can upload databases bigger than 2GB.



A form titled 'New Database' with the following fields and controls:


- Databasename:** A text input field.
- Version:** A text input field.
- File:** A text input field with a 'Browse...' button next to it.
- Description:** A large text area with a vertical scrollbar.
- Create:** A button at the bottom of the form.

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]+)\.*/"/>
URL to the public database to retrieve information:	<input type="text" value="http://eutils.ncbi.nlm.nih.gov/entrez/eutils/efetch.fcgi?db=protein&amp;ret"/>
Parser for the URL information:	<input type="text" value="GBSeqXMLParser"/>

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

[Return](#)

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. In the next line you can specify the URL to the external information fetch page (this URL has to end with 'id=' or whatever your external information page requires, so that the program can add the accession numbers it has to look for) and below the parser for the information page. By default parsers are provided for IPI and GenBank

(although the GenBank parser delivers not so much information as the IPI parser since not so much is available directly). If you want to enhance the existing parsers or write your own parser please visit 2.2.1. .

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 and the links to the external sources at the top:

External data link: <http://eutils.ncbi.nlm.nih.gov/entrez/eutils/efetch.fcgi?db=protein&retmode=xml&id=gi|19114688,gi|1723488,gi|7490714,gi|1213267>

External html link: <http://www.ncbi.nlm.nih.gov/entrez/viewer.fcgi?db=protein&id=gi|19114688,gi|1723488,gi|7490714,gi|1213267>,

Complete Entry:

```
>gi|19114688|ref|NP_593776.1| hypothetical homeobox domain protein [Schizosaccharomyces pombe]
MRSYSNPENGGQINDNINYSKRPTMLPENLSLSNYDMDSFLGQFPDNNMQLPHSTYEQHLQGEQQNPTNPNYFPPEFD
ENKVDWKQEKFPKPDAPSFDNNSFDNVNNSKLTNPSPVQPNIVKSESEFANSKQNEVVEATSVEKAKENVAHESGTPESG
GSTSAPKSKKQLRTADQLAYLLREFSKDTNPPPAIREKIGRELNIPERSVTIWFQNRRAKSKLISRRQEEERQRILREQR
ELDSLQKVSQAFAHEVLSTSPSTPYVGGIAANRQYANTLLPKPTRKTGNFYMKSGPMQSSMEPCIAESDIPRQSLSSST
YYNSLSPNNAVPSQKYSASSYSAIPNAMSVSNAQFDVESPPSSYATPLTGIRMPQPESDLYSYPREVSPSSGGYRMFG
HSKPPSSYKASGFVRPPNMGHMTSSEPTSYDSEFFYFSCITLLVIGLWKRLRASPDLMCFYSPKKLFAYLIQFQGIQ
YRIEYFFVIESIHVFRVEEPLNELSATSSRDKPAPEYWLQMDIQLSVPPVFMITSEGQGNCTDFTEGNQASEVLL
HSLMGRATSMFQMLDRVRASPELGSVIRLQKGLNPHQFLDPQWANQLPRQPDSSVFDHQGRNPPIQGLSHDTSSEYGNK
SQFKRLRSTSTPARQDLAQHLLPKPTNTEGLMHAQSVSPITQAMKSANVLEGSSTRLSNYSVSSAYPHHNLALNLDNT
QFGELGTSNISYPLSAPSDVGSPLPRASNSPSRPVMPHPTQGINTEIKDMAAQFPNSQTGGTLPNSWSMNTNVSVPFTTQN
REFGGIGSSSITMTNAPSQQLSQVFPFGDVSLATENSVPSPSYGFEVPSSESVYAQAARTNSVSVAGVAPRLFIQTPSIPLAS
SAGQDSNLIKSSSGGVYASQPGASGYLSHDQSGSPFEDVYSPSAGIDFQKLRGQQFSPDMQ
```

Rule accession\_rule: gi|19114688,gi|1723488,gi|7490714,gi|1213267,

Rule description\_rule: hypothetical homeobox domain protein [Schizosaccharomyces pombe],Hypothetical

Rule organism\_rule: Schizosaccharomyces pombe,null,null,Schizosaccharomyces pombe,

Complete Entry:

```
>gi|496693|emb|CAA56020.1| B-127 protein [Saccharomyces cerevisiae]
MPFSFLAQFPFPCKISSSTHSLGVNSPGRGSHGNLNVFWYKLSISGLIEEDIVVDSPGFVVVISLLWLVEVGDLILVLPV
AFVPGFATVVPILKLENVFLGDIWFVVDVGLDSSDVLSSIVFIRGL
```

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]
MGKYTKTAILSVYDKTGLDLAKGLVENNVIRILASGGTANMVREAGFPVDDVSSITHAPEMLGGRVKTILHPAVHAGILAR
NLEGDEKDLFEQHIDKVDVFNCLNYPFKETVAKIGVTVQEAVEEIDIGGVTLRLAAAKNHSRVTLISDPNDYSIFLQDLS
KDGEISQDLNRNFALKAFETADYDAAISDFFRKQYSEGKALPLRYGCNPHQRPAQAYITQQEELPFKVLCTPGYINL
LDALNSWPLVKELASLNLPAASFKHVSAGAAVGLPLSDVERQVYFVNDMEDLSPACAYARAGADRMSSFGDFIAL
SNIVDVATAKIIISKEVSDGVIAPGYEPEALNILSKKNGKCYILQIDPNYVPGQMESREVFVGTLLQQRNDIAINQSTFK
EIVSKNKALTEQAVIDLVATILVLKYTQNSVCYAKNGMVVGLGAGQQSRIHCTRLAGDKTDNNWLRQHPKVLNMMKWAKG
IKRADKSNAILDLFTVGQRIEGPEKVDYESKFEVPEPFTKEERLEWLSKLNNVSLSSDAFFFPDPNVYRAVQSGVKFITA
PSGSVMDKVVQAAQDSFDIVYVENPIRLFHH
```

Rule accession\_rule: gi|6323056,gi|1709914,gi|7433574,gi|1480728,gi|2204263,

Rule description\_rule: AICAR transformylase/IMP cyclohydrolase; Ade16p [Saccharomyces cerevisiae],Bif

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). The first line (this will be just there URL and the parser is chosen) is the external link how the data is returned for the parser, the second line is the link which will be put on the accession number in the protein overview (see 7.1)

If 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.

### 2.2.1 Enhanced or self-written parsers plug-in:

MASPECTRAS features a plug-in mechanism to extend the external DB-information fetch. A self-written parser (in a JAR-file) has just to be put in the \$JBOSS\_HOME\$/server/maspectras/sequenceParsers folder to be detected at the next restart of MASPECTRAS. The current implementation provides parsers for IPI and GenBank (here not all of the information available) and therefore there are the IPIParser.jar and the GBSeqXMLParser.jar. The IPIParser can be regarded as show-case of how to implement a self-written parser and therefore it is provided including the source code (IPIParser.java) (in the GBSeqXMLParser the source code is provided as well but rather for self-written enhancements).

The JAR-file must contain the parser class (in binary format), all classes which are required for your parser and the following entry in the META-INF/MANIFEST.MF:

Parser-Class: at.tugraz.genome.maspectras.parser.sequenceInformation.IPIParser.

This is the fully qualified name of your parser class, so that MASPECTRAS knows which Class to instantiate for the parsing. The self-written parsing class has to implement at.tugraz.genome.maspectras.parser.interfaces.SequenceInformationParser interface to be accepted, which can be found in the maspectras.jar. The parsers have to return a Vector<SequenceResultVO>, which contain the identifier of the external plus a description (not mandatory can be 'null' as well). The current implementation allows the fetch of information about:

- Entrez Gene
- Ensembl;
- Ensembl Havanna
- Gen3D
- GO
- NCBI Taxonomy
- InterPro
- PathoSign
- Pfam
- PROSITE
- RefSeq
- SMART
- UniProt-SwissProt
- UniProt-TrEMBL
- Vega
- PubMed
- iHOP
- KEGG

- Gene symbol
- Synonym

If your required web-page does not deliver some of the required information, just return 'new Vector<SequenceResultVO>;' or null. If further information entries are desired please contact the developers at [maspectras@genome.tugraz.at](mailto:maspectras@genome.tugraz.at). It is **important** that the parser can handle the fetch of several entries at once identified by an accession number, since MASPECTRAS fetches always a bundle of 50 entries, since one by one would take too much time. For a detailed documentation of a parser please take a look at the IPIParser.java.

The external fetch strategy itself works like the following:

- HTTP connection to the external data resource you specified in 2.1
- Parsing with a standard parser or your self-written parser
- If a Uniprot-Swissprot entry exists the system makes a connection to Uniprot as well to receive further information (e.g. Pubmed identifiers)
- Parsing of Uniprot files by existing MASPECTRAS parsers

Therefore it is possible that further information is fetched via Uniprot if your parser returns Uniprot identifiers, which is not in the original data file.

## 2.2 File Upload:

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

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](#)

Files per page: 15 [25] 50 100

2 Files found

Page 1 of 1

go to page  go

Nr.	ID	Upload Name	Category	Added Date				
1	251	ICPL_Protmix_1Iizu1he_A_c1	rawdata	2008-02-13				
2	252	ICPL_Protmix_1Iizu1he_A_c1_ms2	mascot	2008-02-13				

Files per page: 15 [25] 50 100

2 Files found

Page 1 of 1

go to page  go[New file upload](#)[New multiple file upload](#)

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

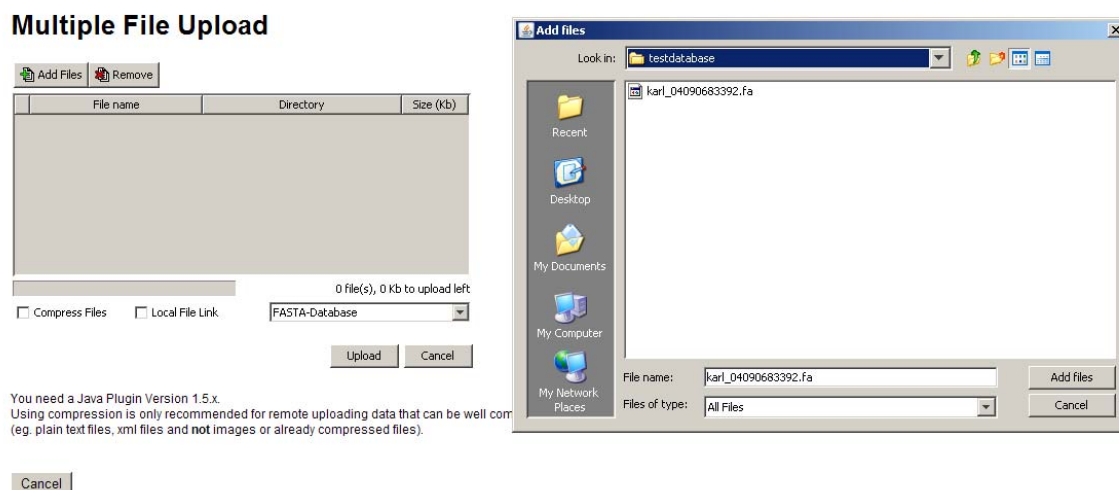
### New File Upload

Name	<input type="text"/>
File	<input type="text"/> <a href="#">Browse...</a>
Local File	<input type="checkbox"/>
File Type	<div><div></div><div></div></div>
Comment	<div>Raw-File MS-Parameters SpectrumMill SpectrumMill Before Version A.03.02 SM Config SM Custom Config <b>Mascot</b> Sequest XITandem Omssa Omssa Modification File CeMM-Internal CeMM Definition File Gel1D Raw Image Gel1D Warped Image Gel1D Annotated Image Gel1D Warping Map Gel2D Raw Image Gel2D Warped Image Gel2D Annotated Image Gel2D Warping Map LC-Column Parameters</div>
Upload	<input type="button" value="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. After the raw file is uploaded an automatic conversion in a more convenient format for the calculation is started (you can see the progress in the upload status page see 2.3). automatically. If this is not desired, there is the option to work directly on one of the formats, but then the real 3D view does not work, just the quasi-3D view (see 7.7). If you want to turn off this feature contact the administrator

of your system. In the file \$DATAROOTDIRECTORY\$/analyses/partitioning/cluster.properties there is an attribute translateChromatograms=true. Set this attribute to translateChromatograms=false. The “Local File” check box is just applicable if the file is on the same system (or mounted on the system) where MASPECTRAS is located. Here no upload is made just a link to the file is stored. Through this file duplication can be avoided and disk space saved.

When you click “New multiple file upload” you come to the multiple file upload applet:



With the “Add Files” a new window opens where you can choose your files and they are displayed in the list below. In the list you can select the files and with “Remove” you can remove them from the list. The “Compress File” option can be used to reduce the transfer over the network but it takes some time to compress and decompress the file again. This option should not be used for already zipped files. Then there is a select box with the categories. There are the same ones like in the normal “New file upload”, plus the category “FASTA-Database”. With this option you can upload databases bigger than 2GB into the system. The database is not displayed in the normal “FileUpload” list but moves directly to the databases (see 2.1). The “Upload” button starts the upload of the selected files. When the upload was successfully finished a green check icon appears in front of the name. When there was an error a red “cross-out” icon appears.

## 2.3 Upload Status:

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

<b>Sample Generation</b>
<b>Management</b>
<b>File Upload</b>
<b>▼ Status Information</b>
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></div></div>	100 %
<input type="checkbox"/>	11851	testKarl22	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	11852	testKarl23	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	11951	F001244	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	12050	F001276	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	13000	Task1ms22400-3600	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	13300	SpectrumMill	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	13301	MascotCompSpectrMill	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	13400	BSA_500fmolH6-1000fmolD6	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	13550	CompToSequest	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	14250	Task2synthDBAll	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	14350	Task2testKarlDB2	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	14450	newMascot	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	14750	MSDB	LOADING FINISHED		<div><div></div></div>	100 %
<input type="checkbox"/>	14850	Task2CompToMasc	LOADING FINISHED		<div><div></div></div>	100 %

Update Interval [m:ss]

## 2.4 Software:




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

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

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"/>	

### Add Upgrade



Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Inserm U255"/>

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  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  go

## 2.5 Dictionary:

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

<b>Sample Generation</b>
<b>Mass Spectrometry</b>
<b>MS-Analysis</b>
<b>Management</b>
<b>File Upload</b>
► <b>Status Information</b>
► <b>Database</b>
► <b>Software</b>
▼ <b>Dictionary</b>
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:

Value:

Description:

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	malidiPlateComposition	stainless steel			✗
8	malidiPlateComposition	coated glass			✗
9	malidiMatrixcomposition	alpha-cyano-4-hydroxycinnamic acid			✗
10	malidiPsdType	PSD			✗
11	malidiPsdType	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.

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

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.

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

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

## New Experiment

Hypothesis:	<input type="text"/>
MethodCitations:	<input type="text"/>
ResultCitations:	<input type="text"/>
Title:	<input type="text"/>
Description:	<input type="text"/>
Show in tree:	<input type="text" value="yes"/> ▼
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Bioinformatics Group"/> ▼

With the “Show in tree” option you can specify if this experiment should be shown in the tree.

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

Experiment

Query
 Edit Display Settings

Experiments per page: 15 [25] 50 100

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

Nr.	Title			
1	testExp			

Experiments per page: 15 [25] 50 100

1 Experiments found
 | Page 1 of 1
 | go to page  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></div></div>

Sampleorigins

Sampleorigin:  

Add Sampleorigin

Owned by User: ☐

Owned by Inst.: ☒

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](#)

### Experiments

Nr.	Title		
1	testNode		✗
2	anotherNode		✗
3	nd		✗
4	notWorkingNode		✗
5	anotherSub		✗

Samples per page: 15 [25] 50

1 Samples found

Page 1 of 1

go to page 

Nr.	SampleId	SampleDate	Title	Description	ProteinAmount			
1	AutomaticFT	2007-07-16	AutomaticFT					✗

Samples per page: 15 [25] 50

1 Samples found


Page 1 of 1

go to page [Add Sub Experiment](#)[Create Sample for Experiment](#)[Add Samples](#)[Compare Results](#)[Return](#)


With the “Add Sub Experiment” you can create a sub-experiment.

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:	<div><div></div></div>

Sampleorigins

Sampleorigin:  

Add Sampleorigin

Owned by User: ☐

Owned by Inst.: ☒ Bioinformatics Group

Create

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

## 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

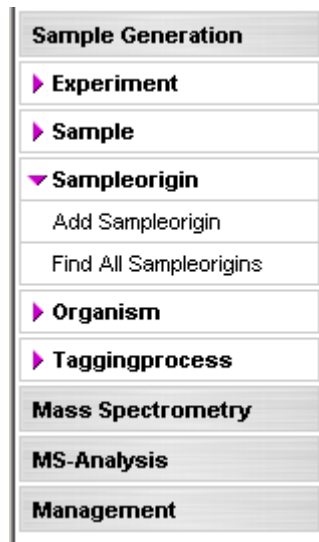
Return

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.



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

## New Sampleorigin

Name:	<input type="text"/>		
Organism:	<input type="text"/>	▼	
Taggingprocess:	<input type="text"/>	▼	
Samplecondition:	<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></div>		
Owned by User:	<input type="checkbox"/>		
Owned by Inst.:	<input checked="" type="checkbox"/>	<input type="text" value="Bioinformatics Group"/> ▼	
<input type="button" value="Create"/>			

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:

Sampleorigins per page: 15 [25] 50 100

1 Sampleorigins found

Page 1 of 1

go to page  go

Nr.	Name	Organism			
1	aGoodOrigin	Human			

Sampleorigins per page: 15 [25] 50 100

1 Sampleorigins found

Page 1 of 1

go to page  go

## 3.4 Organism:

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

<b>Sample Generation</b>
▶ Experiment
▶ Sample
▶ Sampleorigin
▼ Organism
Add Organism
Find All Organisms
▶ Taggingprocess
<b>Mass Spectrometry</b>
<b>MS-Analysis</b>
<b>Management</b>

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

## New Organism

SpeciesName:	<input type="text"/>
StrainIdentifier:	<input type="text"/>
RelevantGenotype:	<input type="text"/>
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Bioinformatics Group"/>

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.

<b>Sample Generation</b>
▶ Experiment
▶ Sample
▶ Sampleorigin
▶ Organism
▼ Taggingprocess
Add Taggingprocess
Find All Taggingprocesses
<b>Mass Spectrometry</b>
<b>MS-Analysis</b>
<b>Management</b>

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

## New Taggingprocess

Name:		
LysisBuffer:	<div></div>	<div></div>
TagType:	<div></div>	<div></div>
TagPurity:		
ProteinConcentration:		
TagConcentration:		
FinalVolume:		
IncubationTime:		
Owned by User:	<input type="checkbox"/>	
Owned by Inst.:	<input checked="" type="checkbox"/>	<div>Bioinformatics Group</div>

Create

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

## Taggingprocess

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

Taggingprocesss per page: 15 [25] 50 100

1 Taggingprocesss found

Page 1 of 1

go to page  go

Nr.	Name			
1	myTaggingProcess			

Taggingprocesss per page: 15 [25] 50 100

1 Taggingprocesss found

Page 1 of 1

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

refresh tree

Sample

Lc Column

Fraction

Fraction

Fraction

Chemical Treatment

Treated Analyte

Gel 2D

Spot

Spot

Sample testSample

Edit Display Settings

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

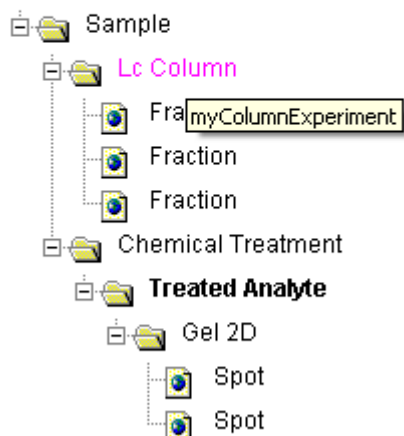
There are 5 different processing methods. A Gel1D leads to bands (for detailed information see chapter 4.2 Gel1D), a Gel2D leads to spots (for detailed information see chapter 4.3 Gel2D), a LC-Column leads to Fractions (for detailed information see chapter 4.4 LC-Column), a Chemical Treatment leads to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

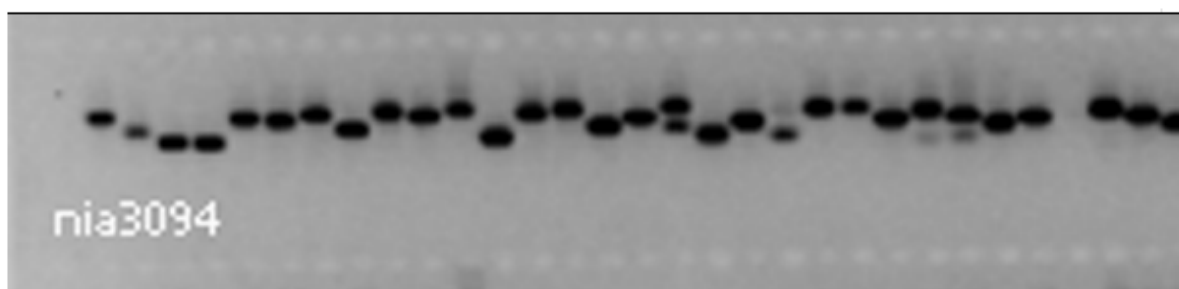
For the “Acquisition Component” you can select the whole selected “Gelmatrix” named with “Main” (you will find this select field, when you click on the “Gel” tab) or one of the components of the “Gelmatrix”. The references to the files (mostly images) which you can select in the “Image” tab, must be 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:	testBoundaryChain		
Area:			?
Intensity:			?
LocalBackground:			?
Annotation:			?
AnnotationSource:			?
Volume:			?
Normalisation:	<input type="text"/>	<input checked="" type="radio"/>	?
NormalisedVolume:			?
LaneNumber:	<input type="text"/>		?
ApparentMass:			?
Description:	<div></div>		
LocalisationItemType:	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"/>	<input type="text" value="[pxs]"/> ✗
Directionstep:	<input type="text" value="SW"/>	<input type="text" value="16"/>	<input type="text" value="[pxs]"/> ✗

**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>	<b>Buffer</b>	<i>Inter Dim.</i>	<i>Spot Detection</i>	<i>Image Acquis.</i>	<i>Image</i>
------------	---------------	-------------------	-----------------------	----------------------	--------------

<b>Buffer X</b>	<b>Buffer Y</b>
-----------------	-----------------

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.

## New Spot

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

Add direction step

Update

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

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 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: otherAnalyteProcessingStep

Update

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:

Create

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

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.

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

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.

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

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:				?		
Acrylamide:bisacrylamide:				?		
Gel Part						
X						
Name:	<input type="text"/>	<input type="radio"/>	?			
X:	<input type="text"/>	Y:	<input type="text"/>	Z:	<input type="text"/>	?
Percentage acrylamide:				?		
Acrylamide:bisacrylamide:				?		
Gel Part						
X						
Name:	<input type="text"/>	<input type="radio"/>	?			
X:	<input type="text"/>	Y:	<input type="text"/>	Z:	<input type="text"/>	?
Percentage acrylamide:				?		
Acrylamide:bisacrylamide:				?		
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.

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

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]
<b>Add a component</b>	
<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			

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

### 4.11 Detection agent

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

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

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:	<input type="text"/>	✖
Specificity:	<input type="text"/>	ⓘ
Species:	<input type="text"/>	
Target:	<input type="text"/>	

**Add antibody**

Create

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

**Detectionagent**
Query
Edit Display Settings

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

Reagents per page: 15 [25] 50 100

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

Reagents per page: 15 [25] 50 100

4 Reagents found | Page 1 of 1 | go to page  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.

<b>Sample Generation</b>
<b>Mass Spectrometry</b>
► <b>Ionsource</b>
► <b>Mzanalysis</b>
► <b>Detection</b>
▼ <b>Massspecmachine</b>
Add Massspecmachine
Find All Massspecmachines
► <b>Controlsoftware</b>
<b>MS-Analysis</b>
<b>Management</b>

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


<b>New Massspecmachine</b>		 Query	 Filter
----------------------------	--	---	--

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></div></div>

Add details for an MS-level

Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/>
	<input type="text" value="Inserm U255"/> 

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 the links at the top for “Filter” and “Query” you can specify machine-specific filters for the upload (see 6.2) or machine specific default filters for the protein/clustered view (see 7.1). With a click on the “Find All Massspectromachines” button you get an overview of all your mass spectrometry machines:

**Massspectromachine**
Query
Edit Display Settings

Massspectromachines per page: 15 [25] 50 100

1 Massspectromachines found

Page 1 of 1

go to page  go

Nr.	Name	ModelName			
1	myMassspectromachine	myModel			

Massspectromachines per page: 15 [25] 50 100

1 Massspectromachines found

Page 1 of 1

go to page  go

## 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

► Massspectromachine

► Controlsoftware

MS-Analysis

Management

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

## New Ionsource

Name:	<input type="text"/>
Type:	<input type="text"/>
Owned by User:	ESI MALDI other
Owned by Inst.:	Bioinformatics Group

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](#)

Ionsources per page: 15 [25] 50 100  
9 Ionsources found | Page 1 of 1 | 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				

Ionsources per page: 15 [25] 50 100  
9 Ionsources found | Page 1 of 1 | 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:			
SolventFlorate:			
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 “Acceleration 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:			
Type:	MALDI		
<b>Plate and Matrix</b>			
PlateComposition:			
MatrixComposition:			
DepositionTechnique:			
<b>Voltage Settings</b>			
GridVoltage:			[V]
<b>Add Accelerationvoltage</b>			
<b>Post Source Decay</b>			
PsdType:			
PsdDescription:			
ExtractionDelayed:	false		
<b>Laser Settings</b>			
LaserType:			
LaserWavelength:			[nm]
LaserPower:			[microJ]
FocusDiameter:			[microm]
AttenuationDetails:			
PulseDuration:			[ns]
ShotFrequency:			[Hz]
AvgNrOfShotsFiredOnSpectrum:			
Owned by User:	<input type="checkbox"/>		
Owned by Inst.:	<input checked="" type="checkbox"/>	Bioinformatics Group	

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:

**Edit Ionsource**

Name:	other
Type:	other
Description:	Description
Owned by User:	<input checked="" type="checkbox"/>
Owned by Inst.:	<input type="checkbox"/> Bioinformatics Group

Return

Update

---

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.

<b>Sample Generation</b>
<b>Mass Spectrometry</b>
► Ionsource
▼ Mzanalysis
Add Mzanalysis
Find All Mzanalysis
► Detection
► Massspecmachine
► Controlsoftware
<b>MS-Analysis</b>
<b>Management</b>

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

## New Mzanalysis

Name:	<input type="text"/>
Type:	<div><div></div><div><div>Ion Optic</div><div>Quadrupole</div><div>Hexapole</div><div>TOF</div><div>Ion Trap</div><div>FT-ICR</div><div>other</div></div></div>
Owned by User:	
Owned by Inst.:	<div></div>
<div>Create</div>	

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	sda1	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:	<input type="text"/>
Type:	<input type="text" value="Ion Optic"/>
Description:	<div><div></div></div>
Collisioncell:	<input type="checkbox"/>
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Bioinformatics Group"/>
<input type="button" value="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:			
Type:	TOF		
ReflectronState:			<input checked="" type="radio"/>
InternalLength:			
Collisioncell:	<input type="checkbox"/>		
Owned by User:	<input type="checkbox"/>		
Owned by Inst.:	<input checked="" type="checkbox"/>	Bioinformatics Group	

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:			
Type:	Ion Trap		
GasType:			<input checked="" type="radio"/>
GasPressure:		[bar]	
RfFrequency:		[Hz]	
ExcitationAmplitude:			
IsolationCentre:			
IsolationWidth:			
FinalMsLevel:			
Collisioncell:	<input type="checkbox"/>		
Owned by User:	<input type="checkbox"/>		
Owned by Inst.:	<input checked="" type="checkbox"/>	Bioinformatics Group	

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:	<input type="text"/>		
Type:	<input type="text" value="other"/>		
Description:	<input type="text"/>		
Collisioncell:	<input checked="" type="checkbox"/>		
GasType:	<input type="text"/>	<input type="button" value="Gas Type"/>	
GasPressure:	<input type="text"/>	<input type="text" value="[bar]"/>	
CollisionOffset:	<input type="text"/>		
CollisionEnergy:	<input type="text"/>		
Owned by User:	<input type="checkbox"/>		
Owned by Inst.:	<input checked="" type="checkbox"/>	<input type="text" value="Bioinformatics Group"/>	
<input type="button" value="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.

<b>Sample Generation</b>
<b>Mass Spectrometry</b>
► <b>Ionsource</b>
► <b>Mzanalysis</b>
▼ <b>Detection</b>
Add Detection
Find All Detections
► <b>Massspecmachine</b>
► <b>Controlsoftware</b>
<b>MS-Analysis</b>
<b>Management</b>

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

New Detection

Name:

Type:

DetectorSensitivity:

RateOfDataAcquisition:

[GHz]

Create

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.

<b>Sample Generation</b>
<b>Mass Spectrometry</b>
▶ <b>Ionsource</b>
▶ <b>Mzanalysis</b>
▶ <b>Detection</b>
▶ <b>Massspecmachine</b>
▼ <b>Controlsoftware</b>
Add Contr.Softws
Find All Contr.Softw.s
<b>MS-Analysis</b>
<b>Management</b>

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

### New Controlsoftware

PackageName:	<input type="text"/>
IsolationWidth:	<input type="text"/>
<b>Criteria</b>	
Criteria:	<input type="text"/>
<b>Add Criteria</b>	
<b>Softwares</b>	
Software:	<input type="text"/>
<b>Add Software</b>	
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> Bioinformatics Group
<input type="button" value="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:

**Controlsoftware**

 Query
 Edit Display Settings

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.

Name:	<input type="text"/>
GenerationDate:	<input type="text"/>
Massspecmachine:	<input type="text"/> 
Control and Analysis Software:	<input type="text"/> 
Parameters File:	<input type="text"/> 
Raw File:	<input type="text"/> 
Description:	<input type="text"/>
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Bioinformatics Group"/>

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:** BSA\_500fmH6\_50fmD6[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_1hzu1	
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.

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). The  $\Delta$  means the allowed threshold difference between the first and the rest of the found hits for one search. The “Min Peptide Length” specifies how many amino acids a peptide must have at least and the “# Peptides for protein” specifies how many peptides have to be found to accept a protein. With the “Alignment” option you can specify if an alignment of the sequence based clustering has to be done by ClustalW. The reason why this option has been made was that it was a time consuming step and that there was much more disk space consumption with the alignment. If you select “NONE” the only thing not possible is the clustered view described at 7.2. The “Just top intensity peaks” option allows the save of disk space. It is specifiable how many (the ones with the best intensity)

should be store (e.g. if you enter 100 the 100 peaks with the highest intensity will be stored in the database while the rest will be discarded).

File Upload

Query
 Edit Display Settings
 Quant-Settings

Sequest Sf Threshold:	0.1	Δ:	1.0
Sequest Peptide Threshold:	+1: 1.5 +2: 2 +3: 2.5	Δ:	1.0
Peptide Prophet Threshold:	0.0	Δ:	1.0
Mascot Peptide Threshold:	+1: 15 +2: 20 +3: 25	Δ:	100
SpectrumMill Peptide Threshold:	10	Δ:	100
SpectrumMill Config File			
SpectrumMill User Config File			
X!Tandem Peptide Threshold:	30	Δ:	1000
Omssa e-Value Threshold:	20	Δ:	1000
Omssa Modification File:			
CeMM InsilicoDef File:			
Min Peptide Length:	5		
# Peptides for protein:	1		
Alignment:	ClustalW		
Just top intensity peaks:	<input type="checkbox"/>		
Quantification tolerance +/-m/z [Da]:	1.0		

save!

Files per page: 15 [25] 50 100

187 Files found | Page 1 of 8 | [Next](#) go to page  go

	Upload Name	Category
<input type="checkbox"/>	Task1ms22400-3601	sequest
<input type="checkbox"/>	MascotMist	mascot
<input type="checkbox"/>	MascProbe1F001927	mascot
<input type="checkbox"/>	PhosphoRealData	mascot
<input type="checkbox"/>	Task3karlDBMS3	sequest
<input type="checkbox"/>	ICPL_Protmix_1lizu1he_A_c1_XTandem	xtandem
<input type="checkbox"/>	ICPL_Protmix_1lizu2he_A_c2_ms2	mascot
<input type="checkbox"/>	ICPL_Protmix_10lizu1he_A_c1_ms2.dat	mascot
<input type="checkbox"/>	ICPL_Protmix_10lizu1he_B_c1_ms2.dat	mascot
<input type="checkbox"/>	ICPL_Protmix_10lizu1he_C_c1_ms2.dat	mascot
<input type="checkbox"/>	ICPL_Protmix_1lizu10he_A_c2_ms2.dat	mascot
<input type="checkbox"/>	ICPL_Protmix_1lizu10he_B_c2_ms2.dat	mascot
<input type="checkbox"/>	ICPL_Protmix_1lizu10he_C_c2_ms2.dat	mascot
<input type="checkbox"/>	ICPL_Protmix_1lizu1he_B_c1_ms2.dat	mascot
<input type="checkbox"/>	ICPL Protmix 1lizu1he C c1 ms2.dat	mascot

>>

<<

Files per page: 15 [25] 50 100

5 Files found | Page 1 of 1 | go to page  go

	Upload Name	Category
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1lSequest	sequest
<input type="checkbox"/>	bsa_1hzu1lXTandem	xtandem
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1lOMSSA	omssa
<input type="checkbox"/>	Mascot1hzu1l	mascot
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1lSpectrumMill.zip	spectrummill

Files per page: 15 [25] 50 100

5 Files found | Page 1 of 1 | go to page  go

The icon opens a new box where you can specify quantification options (if needed):

## File Upload

Query Edit Display Settings Quant-Settings

Sequest Sf Threshold:	0.1	Δ:	1.0
Sequest Peptide Threshold:	+1: 1.5 +2: 2 +3: 2.5	Δ:	1.0
Peptide Prophet Threshold:	0.0	Δ:	1.0
Mascot Peptide Threshold:	+1: 15 +2: 20 +3: 25	Δ:	100
SpectrumMill Peptide Threshold:	10	Δ:	100
SpectrumMill Config File			
SpectrumMill User Config File			
XITandem Peptide Threshold:	30	Δ:	1000
Omssa e-Value Threshold:	20	Δ:	1000
Omssa Modification File:			
CeMM InsilicoDef File:			
Min Peptide Length:	5		
# Peptides for protein:	1		
Alignment:	ClustalW		
Just top intensity peaks:	<input type="checkbox"/>		
Quantification tolerance +/-m/z [Da]:	1.0		

save!

Quant Method: ASAPR Standard

Affected AAs: DE Var: ☐ Mass shift:

1. Partner Time shift: 0 Mass shift: 3.18 ✗

2. Partner Time shift: 0 Mass shift: 0 ✗

Add partner

Accept | Save Settings | Remove Stored Settings

These settings are for the detection of partners which are not identified by MS/MS. With “Quant Method” you can specify the used quantification method. “ASAPR Standard” is the standard ASAPRatio peak detection (works better with Ion Trap data) and “ASAPR Enh. Valley” is the new version (works better with FT and Orbitrap data). In general, the more accurate the mass detection of the mass spectrometer is the more feasible the “ASAPR Enh. Valley”. Then you can specify which amino acids carry the modification (for C-terminus and N-terminus write: C-term or N-term). When you just searched with a fixed modification and you have not found partners than uncheck “Var:” (the meaning is the first partner for the comparison a variable modification). Then in the next line you have to specify the expected mass and time shift to the first partner/fixed modification. It is possible to specify as many partner modifications as you like.

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**QueryEdit Display SettingsQuant-Settings

For Re-Quantification:

Quantification tolerance +/-m/z [Da]:


Dbsearchparameterss per page: 15 [25] 50 100

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

Nr.	UploadName	PrepSteps			
<input checked="" type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1ISequest	Sample: compareQuantification			
<input checked="" type="checkbox"/>	bsa_1hzu1IXTandem	Sample: compareQuantification			
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1IOMSSA	Sample: compareQuantification			
<input checked="" type="checkbox"/>	Mascot1hzu1I	Sample: compareQuantification			
<input type="checkbox"/>	060606FTc2_phosphb_bsa_1hzu1ISpectrMill.zip	Sample: compareQuantification			

Dbsearchparameterss per page: 15 [25] 50 100


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


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

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

Return

Update

The  icon restarts the quantification of an uploaded file. After clicking you have to watch the upload status page to see the progress (see 2.3). If there is no raw file specified the icon is greyed out.

The  icon fetches or re-fetches the external information. The icon is greyed out if the corresponding information about the external sources is not given (see 2.1). If you want to know how to display the external information see chapter 7.4.

## 7.1 Protein comparison:

**Protein**QueryEdit Display Settings

1 = 060606FTc2\_phosphb\_bsa\_1hzu11 (Partitioning [\[P\]](#))  
2 = 060606FTc2\_phosphb\_bsa\_1hzu10mssa (Partitioning [\[P\]](#))  
3 = 060606FTc2\_phosphb\_bsa\_1hzu10request (Partitioning [\[P\]](#))  
4 = 060606FTc2\_phosphb\_bsa\_1hzu10ctandem (Partitioning [\[P\]](#))

Proteins per page: [15](#) [25](#) [50](#) [100](#)  
17 Proteins found | Page 1 of 1 | go to page  go

Nr.	Search	AccessionNum	Organism	GeneName	SequCovMax	Score	Nr. of Proteins	Amount of Peptides	
1	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a> <a href="#">4</a>	gi231300		Glycogen Phosphorylase b (E.C.2.4.1.1) (T State) Complex With AMP	53.97	51846.45	1	84	<a href="#">[i]</a>
2	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a> <a href="#">4</a>	gi182648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	2	40	<a href="#">[i]</a>
3	<a href="#">1</a> <a href="#">4</a>	gi435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	355.40	7	9	<a href="#">[i]</a>
4	<a href="#">1</a> <a href="#">2</a> <a href="#">4</a>	gi136429		Trypsin precursor	68.3	237.20	3	6	<a href="#">[i]</a>
5	<a href="#">4</a>	gi11967711	Homo sapiens	anaphase promoting complex subunit 1-Tsg24 protein [Homo sapiens]	5.92	154.00	1	4	<a href="#">[i]</a>
6	<a href="#">4</a>	gi31560568	Mus musculus	MAD homolog 2 [Mus musculus]	7.29	95.30	1	3	<a href="#">[i]</a>
7	<a href="#">4</a>	gi295721	Gallus gallus	conalbumin [Gallus gallus]	5.11	70.00	1	2	<a href="#">[i]</a>
8	<a href="#">4</a>	gi124280		H3_X0	20.0	73.30	5	2	<a href="#">[i]</a>
9	<a href="#">4</a>	gi4885281	Homo sapiens	glutamate dehydrogenase 1 [Homo sapiens]	3.41	77.09	1	2	<a href="#">[i]</a>
10	<a href="#">4</a>	gi124286		DegP (Arabidopsis thaliana)	8.46	70.20	1	2	<a href="#">[i]</a>
11	<a href="#">4</a>	gi4505573		Structural maintenance of chromosome 1-like 1 protein (SMC1alpha protein) (SB1.8/CD/S423E protein) (SB1.8) - Homo sapiens (Human).	5.11	83.70	1	2	<a href="#">[i]</a>
12	<a href="#">4</a>	gi27542557	Homo sapiens	EVIC2 protein variant [Homo sapiens]	2.06	68.59	2	2	<a href="#">[i]</a>
13	<a href="#">4</a>	gi124319		MBP_Bora	3.97	45.90	1	1	<a href="#">[i]</a>
14	<a href="#">4</a>	gi1083952		subtilisin-lysozyme inhibitor, SIL13 - Streptomyces galbus [MAS=10982]	21.11	38.70	1	1	<a href="#">[i]</a>
15	<a href="#">4</a>	gi124230		human pds5 (h EST: Z42154 and fragment: KIAA0648 plus HeLa N-term cDNA; see E Vorlauffer, Ph.D thesis 2002, pp. 49)	1.72	35.40	1	1	<a href="#">[i]</a>
16	<a href="#">4</a>	gi8250019		beta-galactosidase [Cloning vector pBRINT-TsCm]	2.77	35.40	1	1	<a href="#">[i]</a>
17	<a href="#">4</a>	gi8322830	Saccharomyces cerevisiae	Cdc16p [Saccharomyces cerevisiae]	1.43	44.80	1	1	<a href="#">[i]</a>




Proteins per page: [15](#) [25](#) [50](#) [100](#)  
17 Proteins found | Page 1 of 1 | go to page  go

[Export Current View:](#) [Excel](#) [DOC](#) [TEXT](#)

[To Protein View >>](#)  
[To Peptide View >>](#)



Below the header the searches that you have selected are listed by 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 (7.5). 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.

1 = 060606FTc2\_phosphb\_bsa\_1hzu1lSquest (Partitioning ) 2 = bsa\_1hzu1lXTandem (Partitioning ) 3 = Mascot1hzu1l (Partitioning )

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

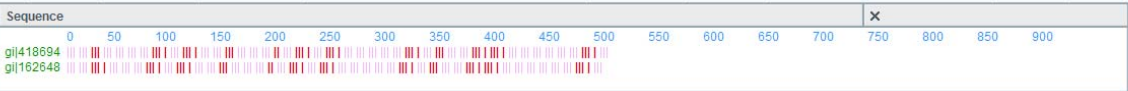
4 Proteins found | Page 1 of 1 | go to page  [go](#)



Nr.	Search	AccNr	Organism	GeneName	%SeqMax	Score	# Prots	# Peps	# Spec	
1	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a>	gi 231300		Glycogen Phosphorylase b (E.C.2.4.1		53.97	2840.53	1	64	952 
2	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a>	gi 418694	validated	serum albumin precursor [validated]		38.06	1308.19	2	26	543 

Details from

Nr.	Search	AccNr	Organism	GeneName	%SeqMax	Score	Cluster Nr.	# Peps	# Spec
1	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a>	gi 418694	validated	serum albumin precursor [validated]	35.59	1308.19	Cluster-1 Cluster-7 Cluster-3	26	543
2	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a>	gi 162648	Bos taurus	albumin [Bos taurus]	1.65	1308.19	Cluster-1 Cluster-7 Cluster-3	26	319

Sequence



3	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a>	gi 999627		Chain B, Porcine E-Trypsin (E.C.3.4		68.3	199.20	3	3	12 
4	<a href="#">1</a> <a href="#">3</a>	gi 1346343		Keratin, type II cytoskeletal 1 (Cy		13.2	337.19	2	1	2 

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

4 Proteins found | Page 1 of 1 | go to page  [go](#)

Export Current View: [Excel](#) | [DOC](#) | [TEXT](#) | [PRIDE XML](#)


[To Protein View >>](#)

[To Peptide View >>](#)


[Return](#)


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.

1 = 060606FTc2\_phosphb\_bsa\_1hzu1l (Partitioning )

2 = 060606FTc2\_phosphb\_bsa\_1hzu1lOmssa (Partitioning )

3 = 060606FTc2\_phosphb\_bsa\_1hzu1lSquest (Partitioning )

4 = 060606FTc2\_phosphb\_bsa\_1hzu1lXTandem (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	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a> <a href="#">4</a>	gi 231300		Glycogen Phosphorylase b (E.C.2.4.1.1) (T State) Complex With AMP	53.97	51846.45	Cluster-4 Cluster-4 Cluster-3 Cluster-11	84
2	<a href="#">1</a> <a href="#">2</a> <a href="#">3</a> <a href="#">4</a>	gi 418694	validated	serum albumin precursor [validated] - bovine	40.37	30102.72	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
3	<a href="#">1</a> <a href="#">2</a> <a href="#">4</a>	gi 162648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
4	<a href="#">4</a>	gi 435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	355.40	Cluster-1	9
5	<a href="#">4</a>	gi 1346343		Keratin, type II cytoskeletal 1 (Cytokeratin 1) (K1) (67 kDa cytoke	13.2	337.19	Cluster-2 Cluster-2 Cluster-4 Cluster-1	8
6	<a href="#">4</a>	gi 39794653	Homo sapiens	Keratin 1 [Homo sapiens]	13.2	337.19	Cluster-2 Cluster-2 Cluster-1	8
7	<a href="#">4</a>	gi 71528		keratin 10, type I, cytoskeletal - human	18.39	245.30	Cluster-1	7

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

7 Proteins found | Page 1 of 1 | go to page  [go](#)

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 7.5 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

In the protein list the quantification of the proteins can be displayed, when you click on the  button.

Protein

Query
 Edit Display Settings
 Quant-Settings

☐ STY\*: 79.96
 ☒ C-termDE@: 3.01
 ☐ M%: 15.99
 ☒ no mod

Lower Threshold 1:

0.5

Upper Threshold 1:

2.0

CV% Warning:

60.0

Lower Threshold 2:

0.2

Upper Threshold 2:

5.0

CV% Threshold:

400.0

Amount of needed peptides:

1

☒ Normalize
 ☒ Remove incompletely modified

Accept | Save Settings | Remove Stored Settings

1 = dta and out pool 2\_50 mM\_light (Partitioning

Proteins per page: 15 [25] 50 100

352 Proteins found | Page 1 of 15 | Next >>

go to page  go

Nr.	Search	AccNr	@ID	Organism	GeneName	%SeqMax	Score	# Prots	# P
1	1	gi 5821151 dbj BAA83717.1	1.5669699 CV=55.130905%	Homo sapiens	RNA binding protein [Homo sapiens]	7.14	26.17	3	
2	1	gi 114555524 ref XP_001168085.1	0.8415438 CV=6.7873898%	Pan troglodytes	PREDICTED: thyroid hormone receptor	6.08	18.36	2	
3	1	gi 415819 emb CAA46519.1	!!!0.79695255 !!!CV=70.76151%	Homo sapiens	antigen of the monoclonal antibody	2.09	15.60	1	
4	1	gi 42542379 ref NP_005830.2	0.78091544 CV=38.153564%	Homo sapiens	serine/arginine repetitive matrix 1	4.32	13.68	1	
5	1	gi 7020584 dbj BAA91188.1	0.7862717 CV=42.231552%	Homo sapiens	unnamed protein product [Homo sapie	17.32	11.09	1	
6	1	gi 16553793 dbj BAB71593.1	1.6370167 CV=27.865332%	Homo sapiens	unnamed protein product [Homo sapie	5.98	12.45	2	
7	1	gi 61743954 ref NP_001611.1	0.9607701 CV=2.0296743%	Homo sapiens	AHNAK nucleoprotein isoform 1 [Homo	0.48	7.73	2	
8	1	gi 14141152 ref NP_005959.2	0.62812227 CV=35.785873%	Homo sapiens	heterogeneous nuclear ribonucleopro	5.48	10.33	2	
9	1	gi 5174525 ref NP_005900.1	1.2902057 CV=0.2199976%	Homo sapiens	microtubule-associated protein 1B i	1.99	9.04	1	
10	1	gi 5032189 ref NP_005648.1	!!!2.749998 !!!CV=137.99057%	Homo sapiens	tumor protein p53 binding protein,	1.53	9.99	1	
11	1	gi 56749088 sp Q86UE4 LYRIC_HUMAN	0.5410007 CV=NaN%		Protein LYRIC (Lysine-rich CEACAM1	5.68	8.45	1	
12	1	gi 6382079 ref NP_006258.2	1.1291128 CV=NaN%	Homo sapiens	RAN binding protein 2 [Homo sapiens	1.2	9.87	3	
13	1	gi 3043596 dbj BAA25462.1	!!!1.0410606 !!!CV=121.94556%	Homo sapiens	KIAA0536 protein [Homo sapiens] [MA	3.41	11.40	8	
14	1	gi 21758470 dbj BAC05308.1	0.8461221 CV=NaN%	Homo sapiens	unnamed protein product [Homo sapie	3.26	5.33	1	
15	1	gi 87196351 ref NP_001347.3	1.2410626 CV=NaN%	Homo sapiens	DEAD/H (Asp-Glu-Ala-Asp/His) box po	2.57	4.96	4	
16	1	gi 56118310 ref NP_073568.2	0.42143118 CV=NaN%	Homo sapiens	nuclear ubiquitous casein kinase an	8.65	5.82	1	

In the first line of the quantification box you have to specify the modifications with have to be compared (in this example a fixed modification is selected, therefore “no mod”, against a modification at C-termDE with the value of 3.01). Then you can specify two thresholds to display deviations from the 1:1 ratio in colour. “Normalize” means that a total ratio over all of the peptides is calculated to see if there are any differences in the labelling efficiency and the other values are corrected automatically with this value. This option takes a little bit longer since a lot of peptides have to be fetched from the database. The option “Remove incompletely modified” removes all peptides which do not carry a modification on all of the possible positions. If you want to measure incompletely modified peptides do not use this option.

There is a link on the ratio of the comparison which leads directly to the quantitative peptide overview for this protein (see 7.8).

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

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

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

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

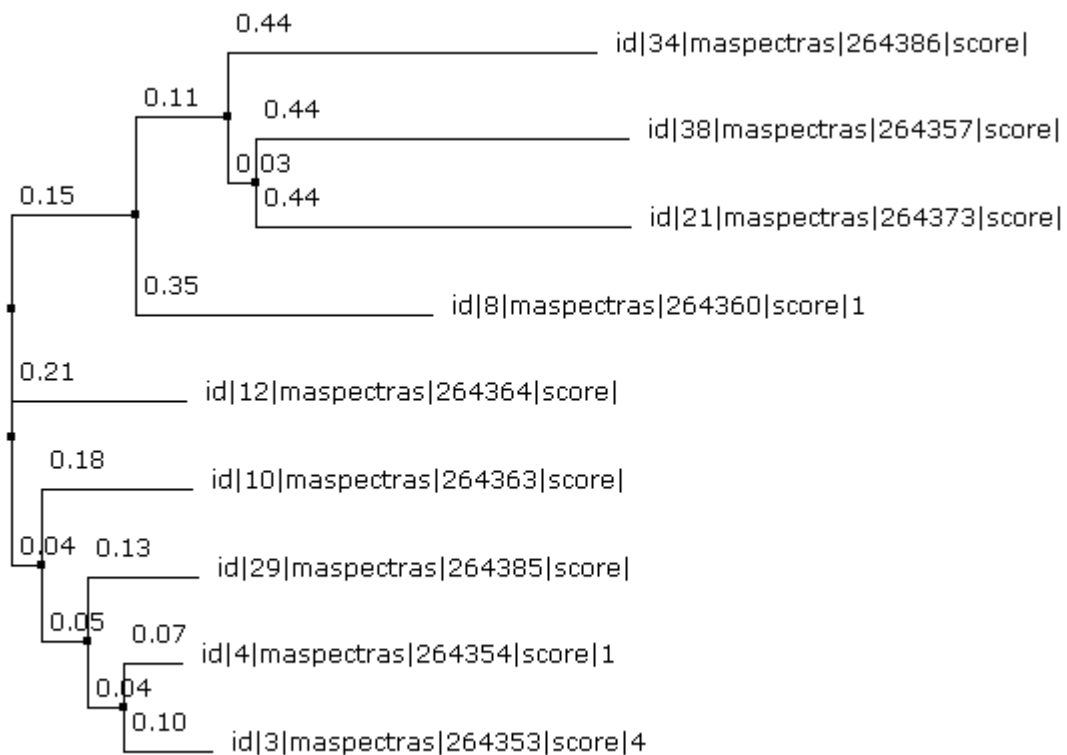
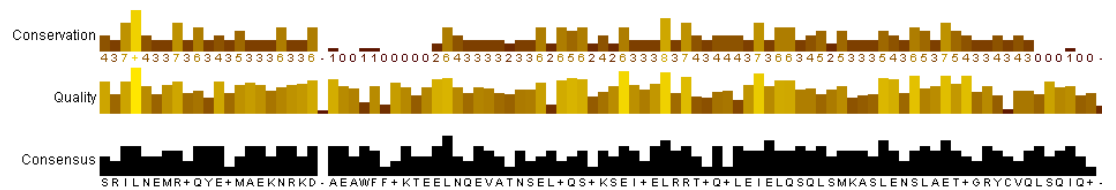
: Download the storage of the tree that you can see in Jalview at the end of this section

: 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 Q 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 M R S Q 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 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 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 Clustering possibilities in MASPECTRAS:

The clustering settings in the clustered protein view can be made in the “Edit Display Settings”. Generally it is possible to select clustering based on the protein sequence (the possibility to show the alignment of the cluster is described at 7.2) or based on mass spectrometry evidence. Since the mass spectrometry evidence based calculated on the fly, no pre-calculation of the alignment is possible. Therefore the quick alignment algorithm KAlign has been included.

**Protein**

Proteins per page: 15 [25] 50 100

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

Nr.	AccNr	Organism	GeneName	Gene Symbol	Domains	%SeqMax	Score	# Prots	# Peps	# Spec		Load	Enz	Ens	PbMd	SPrt
1	IPI00383296.5		Isoform 2 of Heterogeneous nuclear	HNRNPM	RRM	15.78	352.22	2	9	10		Load		e!	Polype	SPrt
2	IPI00220327.3		Keratin, type II cytoskeletal 1	KRT1		11.81	254.10	1	7	7		Load		e!	Polype	SPrt
3	IPI00019359.3		Keratin, type I cytoskeletal 9	KRT9		9.8	197.00	1	4	4		Load		e!	Polype	SPrt
4	IPI00383111.2		57 kDa protein	KRT10		5.42	96.61	6	3	3		Load		e!	Polype	SPrt
5	IPI00021304.1		Keratin, type II cytoskeletal 2 epi	KRT2		4.97	99.76	1	3	3		Load		e!	Polype	SPrt
6	IPI00414676.6		Heat shock protein HSP 90-beta	HSP90AB1	HATPase_c	4.98	128.19	8	3	3		Load		e!	Polype	SPrt
7	gi1136429		Trypsin precursor			12.13	133.87	1	2	3		Load		e!	Polype	SPrt
8	IPI00604620.3		Isoform 1 of Nucleolin	NCL	RRM	3.39	84.62	4	2	2		Load		e!	Polype	SPrt

Proteins per page: 15 [25] 50 100

8 Proteins found

Export Current View: Excel | DOC

To Protein View >>

To Peptide View >>

Return

http://localhost:23080/maspectras/FileProvider?FilePath=%5C%5CMajestix%2FPrj-M5-Analysis%2Fmaspectras%2FData...

File Edit Select View Format Colour Calculate Help

310 320 330 340 350 360 370

IPI00383111/1-564 EELAYLKKNNHEEEMD L RNVSTG D VNVEMN A A P G V D L T Q L L N N M R S Q 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

IPI00009865/1-593 EELAYLKKNNHEEEMD L RNVSTG D VNVEMN A A P G V D L T Q L L N N M R S Q 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

IPI0037591/1-450 EEMTYLKKNNKEEMD V L C C A A G G N V N V E M N A A P G V D L T V L L N N M R A E Y E A L A E Q N R R D A E A W F N E K S A S L Q Q Q I S

IPI00328103/1-469 EELAYLKKNNHEEEMD L Q C C A A G G N V N V E M N A A P G V D L V L L N N M R A E Y E A L A E Q N R R D A E A W F N E K S A S L Q Q Q I S

IPI00743715/1-464 EEMTYLKKNNHEEEMD L Q C C A A G G N V N V E M N A A P G V D L V L L N N M R A E Y E A L A E Q N R R D A E A W F N E K S A S L Q Q Q I S

IPI00418663/1-486 EEMTYLKKNNHEEEMD L Q C C A A G G N V N V E M N A A P G V D L V L L N N M R A E Y E A L A E Q N R R D A E A W F N E K S A S L Q Q Q I S

The procedure to display the alignment is similar to 7.2. First the “Load” button has to be pressed to start the alignment. When the Java icon appears you can click on it and the Jalview Alignment editor will be started to show the results.

The system has further the ability to invoke more than one clustering sequentially (e.g. first the proteins are clustered by MS evidence and then by the sequence). Further clustering methods are planned in future.

Ensembl | ☒ Peptide | ☒ Gen3D | ☒ Pathway | ☒ InterPro

1. Clustering: **Masspec Evidence** 2. Clustering: **Protein Sequence** X

Update | [Display all](#) | [Display default](#) Save Settings

Proteins per page: 15 [25] 50 100 go to page 00

5 Proteins found | Page 1 of 1

Nr.	AccNr	Organism	GeneName	Gene Symbol	Domains	%SeqMax	Score	# Prots	# Peps	# Spec	Enz	Ens	PbMId	SPrt
1	IP100383296.5		Isoform 2 of Heterogeneous nuclear	HNRNPM	RRM	15.78	352.22	1	9	10				
2	IP100220327.3		Keratin, type II cytoskeletal 1	KRT1		11.81	254.10	<b>4</b>	7	7				

Details from

Nr.	AccNr	Organism	GeneName	Gene Symbol	Domains	%SeqMax	Score	# Prots	# Peps	# Spec	Enz	Ens	PbMId	SPrt
1	IP100220327.3		Keratin, type II cytoskeletal 1	KRT1		11.81	254.10	1	7	7				
2	IP100019359.3		Keratin, type I cytoskeletal 9	KRT9		9.8	197.00	1	4	4				
3	IP100383111.2		57 kDa protein	KRT10		5.42	96.61	<b>5</b>	3	3				

Details from

Nr.	AccNr	Organism	GeneName	Gene Symbol	Domains	%SeqMax	Score	# Prots	# Peps	# Spec	Enz	Ens	PbMId	SPrt
1	IP100383111.2		57 kDa protein	KRT10		5.42	96.61	3	3	3				
2	IP100009855.1		Keratin, type I cytoskeletal 10	KRT10		5.06	95.61	3	3	3				
3	IP100375911.2		Type I inner root sheath specific k	KRT25		4.0	44.51	2	2	2				
4	IP100328103.2		Keratin-27	KRT27		3.93	44.51	2	2	2				
5	IP100743715.3		Keratin 25D	KRT28		3.88	44.51	2	2	2				
6	IP100418663.3		Keratin-28	KRT28		3.71	44.51	2	2	2				

Sequence

0 50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900

IP100383111.2  
IP100009855.1  
IP100375911.2  
IP100328103.2  
IP100743715.3  
IP100418663.3

Peptide Sequence X

FSSSSGYGGGSSR  
.GGSGSYGGGSGGGYGGGSGSR  
.SGGGGGGLGGGSGSR  
.TLIDINR

This example shows a protein list which is first clustered by the mass spectrometry evidence and then by the protein sequence. The second row has been expanded with the blue button and the content of the cluster (4 proteins) is shown (clustering by protein sequence). The protein at row three of the cluster is again the representative of a cluster (clustered by MS evidence) which is again expanded by the blue button. The fourth element of the first extended cluster will be continued after the extension of the cluster with second cluster with six elements. Additionally this view has the ability to show the peptides of a specific protein at the right side if you click on the number in the column “# Peps”.

## 7.4 External information:

The system provides the possibility to directly link the found proteins to many external sources. If you want to know how to configure the system to fetch the necessary external information please visit section 2.1 and how you restart just the fetch (and not to do a removal of the uploaded data and start the upload again) please visit section 7 at the beginning.

The fields that should be shown can be set in the “Edit Display Settings” of the page. If you hover the mouse over an external link a popup will open, where there are links to external information. Normally the link is displayed by its ID while in some cases like PubMed the description of link (in this case the title) is getting displayed. On the accession number of the protein is a link on the primary fetch page for the external links (in the example below IPI).

Protein

Query

Edit Display Settings

Quant-Settings

Available fields

Required Information

☒ AccessionNum

☐ Synonyms

☐ Description

☐ PredictedPi

☐ Cluster Nr.

☐ Gene Symbol

☒ GeneName (small)

☐ Organism

☐ Sequence

☐ SequCovMax

☐ Search

☐ Domains(SMART)

☐ GeneName

☐ Amount of Peptides

☐ Modifications

☐ Score

☐ OrfNumber

☐ Hide Keratin

☐ Amount of Spectra

☐ PredictedMass

☒ Nr. of Proteins

☐ Quantification

External links

☒ EntrezGene

☒ GO

☒ iHop

☒ UniprotSwissprot

☒ Vega

☒ Prosite

☒ Ensembl

☒ Pfam

☒ Kegg

☒ UniprotTrembl

☒ NCBI TaxID

☒ RefSeq

☒ EnsemblHavana

☒ Pubmed

☒ Gen3D

☒ PathoSign

☒ InterPro

☒ GeneCard

1. Clustering:

Massspec Evidence

Add Clustering

Update

Display all

Display default

Save Settings

10 Proteins found

Page 1 of 1

Proteins per page: 15 [25] 50 100

go to page go

Nr.	AccNr	GeneName	# Prots		Enz	Ens	Hav	Go	Pfm	PbMd	iHop	Keg	G3D	SPrt	Trbl	PSgn	Vga	TxId	IPro	PrSt	RSq	GCd
1	gi 162648	albumin [Bos taurus]	6																			
2	IPI00440493.2	ATP synthase subunit alpha, mitocho	4																			
3	IPI00479186.5	Isoform M2 of Pyruvate kinase isozy	10																			
4	IPI00219005.3	FK506-binding protein 4	1																			
5	IPI00796844.1	Full-length cDNA clone CS0CAP007YF1	8																			
6	IPI00807545.1	Isoform 3 of Heterogeneous nuclear	4																			
7	gi 136429	Trypsin precursor	1																			
8	IPI00295400.1	Tryptophanyl-tRNA synthetase, cytop	2																			
9	IPI00025252.1	Protein disulfide-isomerase A3 prec	3																			
10	IPI00290110.5	Programmed cell death protein 4	2																			

10 Proteins found

Page 1 of 1

Export Current View: Excel DOC TEXT PRIDE XML

Pubmed >> GeneSymbol

Pubmed >> GeneSynonym

Pubmed

Specific binding of tetratricopeptide repeat proteins to the C-terminal 12-kDa domain of hsp90

Molecular cloning of cDNA encoding a human heat-shock protein whose expression is induced by adenovirus type 12 E1A in HeLa cells

Nucleotide sequence of a full-length cDNA for 90 kDa heat-shock protein from human peripheral blood lymphocytes

SMYD3 encodes a histone methyltransferase involved in the proliferation of cancer cells

Phosphoproteomic analysis of the human pituitary

### 7.5 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 SRGVFRDR DTHKSEIAHRFKDLGEEQFKGLVLIAFSQYLQQCPFDEHV KLVNE
LTEFAKT CVADES HAGCEKSLHTLF GDELCKVASLR ETYGDMADCC EKQEPERNECFLSHKDDSPDLPKL
KPD PNTLCDEFKADEKKFWGKYLYE IARRHPYFYAPE LLYANKYNGVFQDCCQAEDKGACLLPKIETMR
EKVLASSARQLRRCASIQKFGERALKAWSVARLSQKFPKAEFVEVT KLVDLT KVHKECCHGD LLECA DD
RADLAKYICDNQDTISSKLKECCDKP LLEKSHCIAEVEKDAIPENLPPLTADF AEDKD VCKNYQEAKDAF
LG SFLYEYSRRHP EYAVSVLLRLAKE YEATLEECCA KDDPHACYSTVFDK LKHLVDE PQNLIKQNCDQFE
KLGEYGFQNALIVRYTRKVPQVSTPTLVEVS RSLGKVGT RCCTKPESERMPCTED YLSLILNRLCVLHEK
TPVSEKVT KCCTESLVNRRPCFSALT PDETYVPKAFDEKLF TFHADICTLPDTEK QIKKQTALVELLKHK
PKATEEQ LKTVMENFVAFVDKCCAA DDKEACFAVEG PKLVVSTQTALA
```

☐ 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 >>](#)
Peptidehits per page: [15](#) [\[25\]](#) [50](#) [100](#)

go to page  [go](#)

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


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 7.8).

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 7.6).

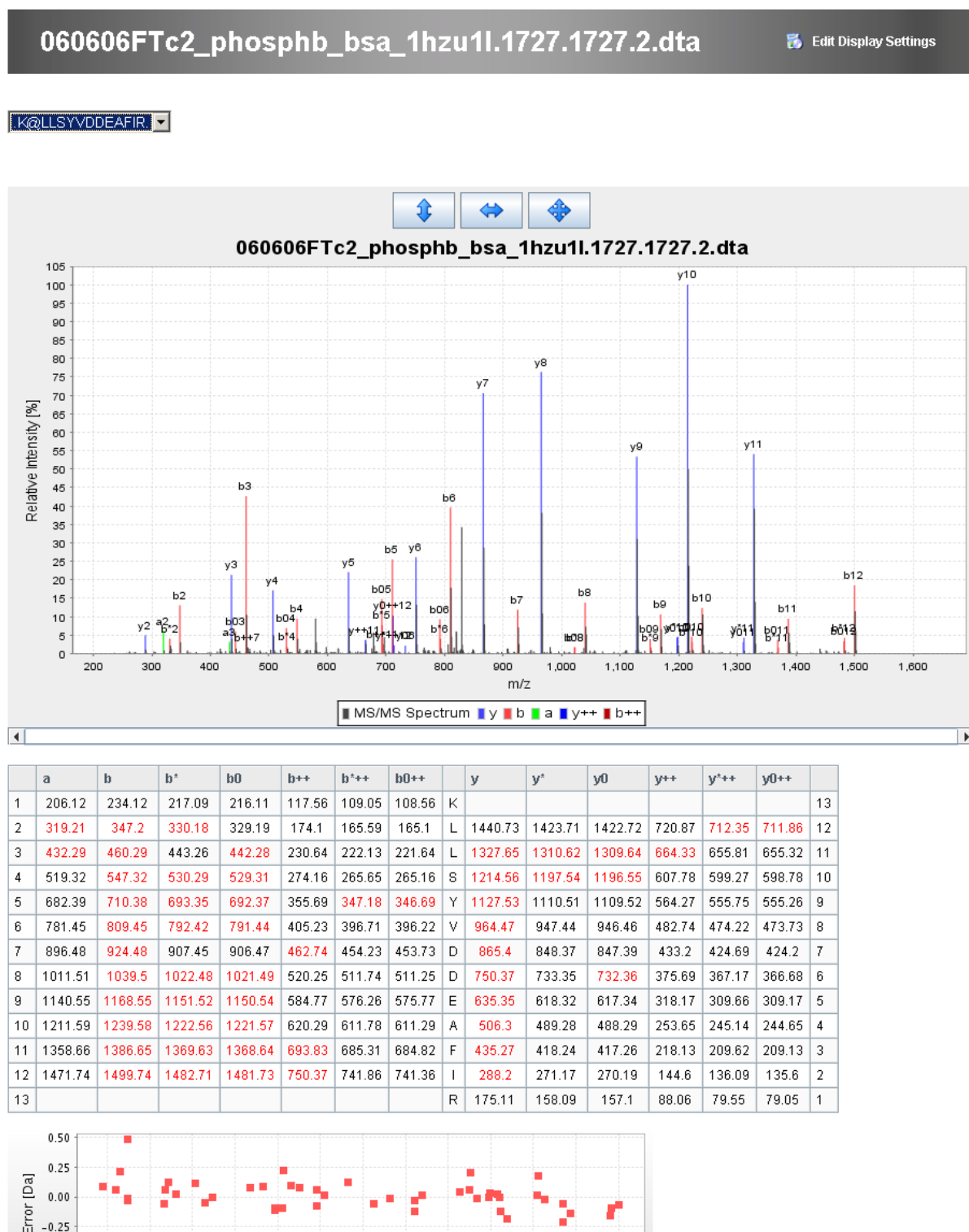
When you click on the link on the peak area entries you receive a chromatogram viewer for the manual inspection and correction of the automatically calculated peak areas (see 7.7.)

#### 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

## 7.6 Spectrum View:

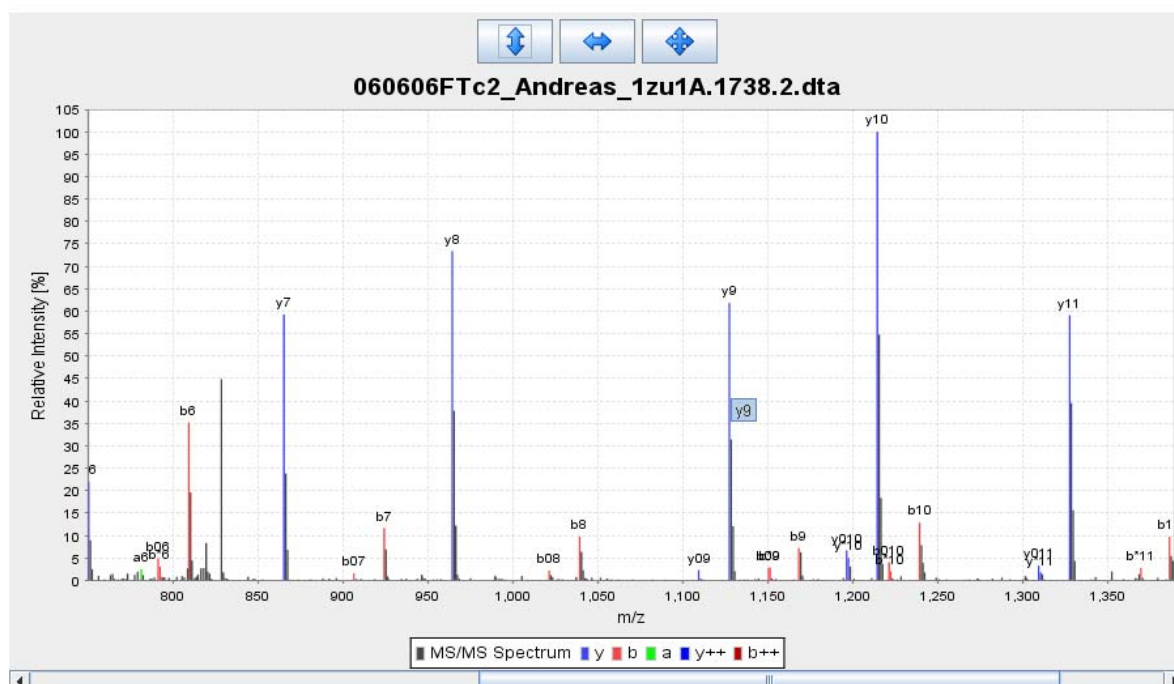


With “Edit Display Settings” you can select the series you want to be displayed. You can save your own display settings like in all the other pages.

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 7.6.1) 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.

### 7.6.1 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

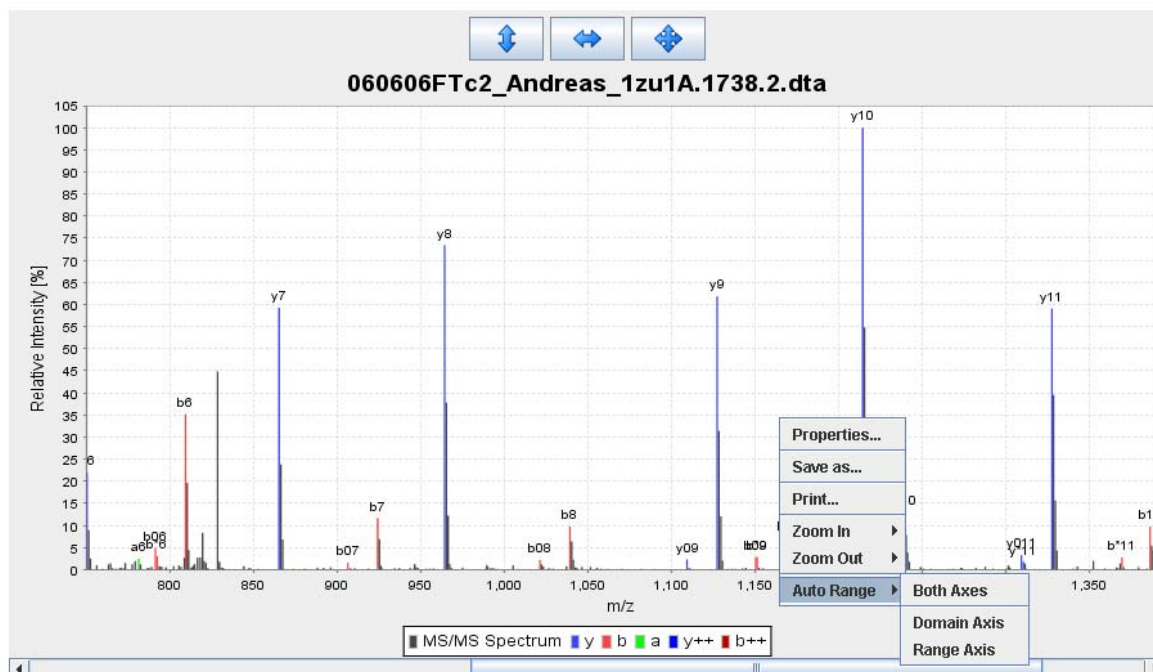


: zooms out the x-axis

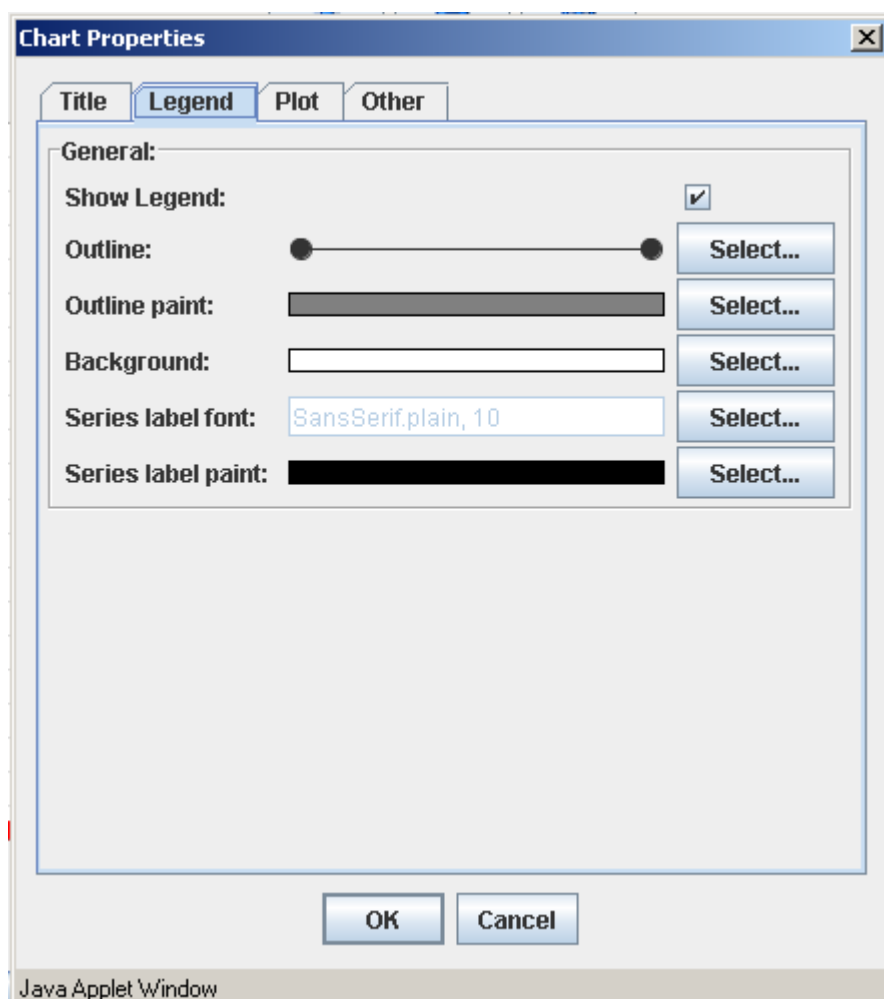


: zooms out both axes

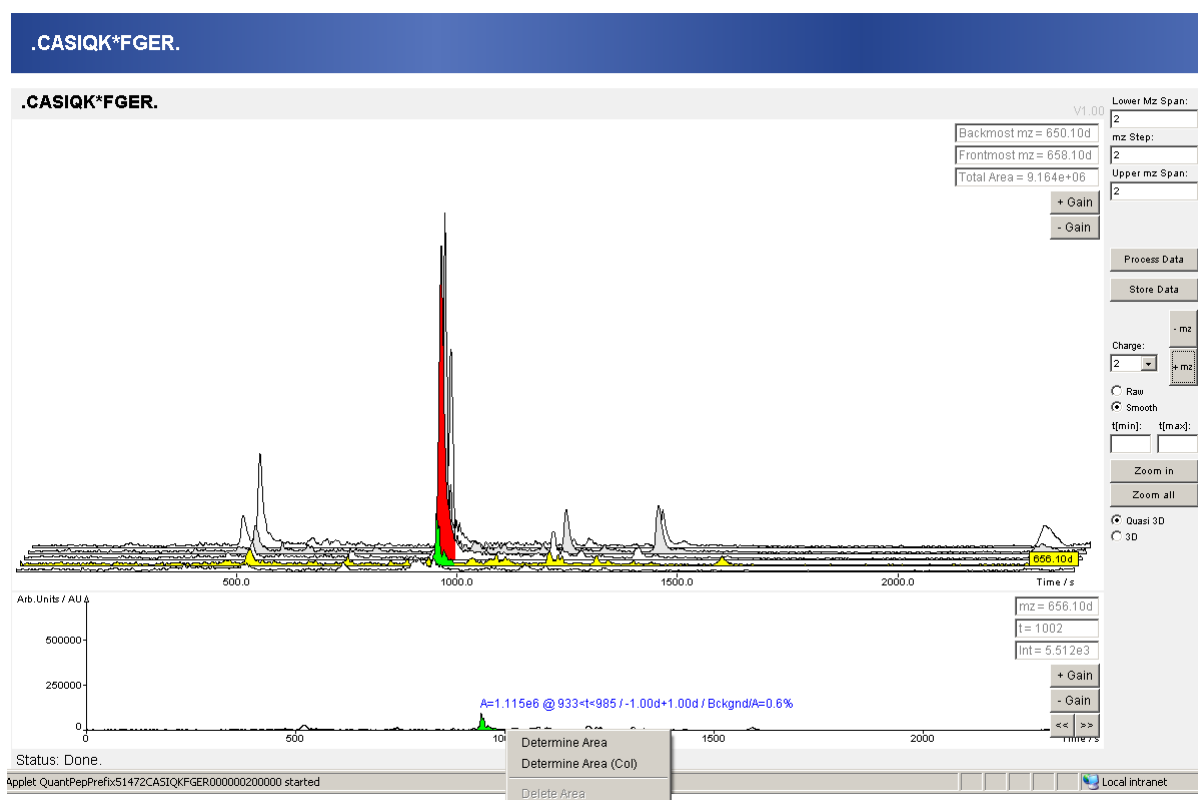
When you first click on the spectrum and then click with the right mouse button you will get a popup window where you have additional features:



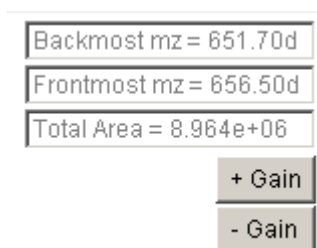
You can print your actual zoom scan. In the “Properties...” you can customize your font and other settings.



## 7.7 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.

Lower Mz Span:

mz Step:

Upper mz Span:

Charge:

☐ Raw  
☒ Smooth

t[min]:   
t[max]:

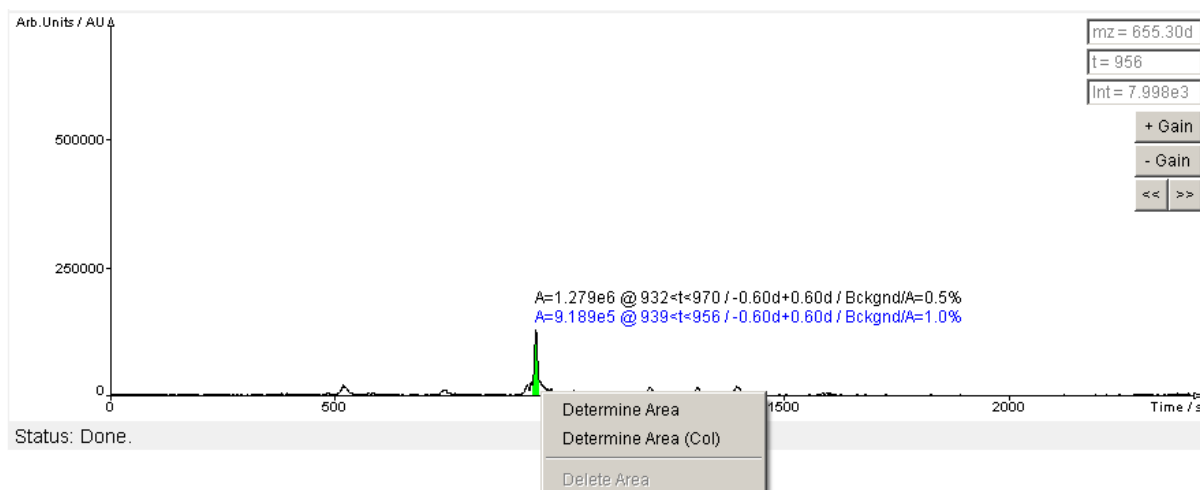
☒ Quasi 3D  
☐ 3D

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. The last check-box changes the quasi-3D view to real 3D viewer. The problem is that the real 3D viewer needs Java3D installed on the client machine and needs much more main memory on the machine (see 7.7.1)

mz = 655.30d  
t = 956  
Int = 7.998e3

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.



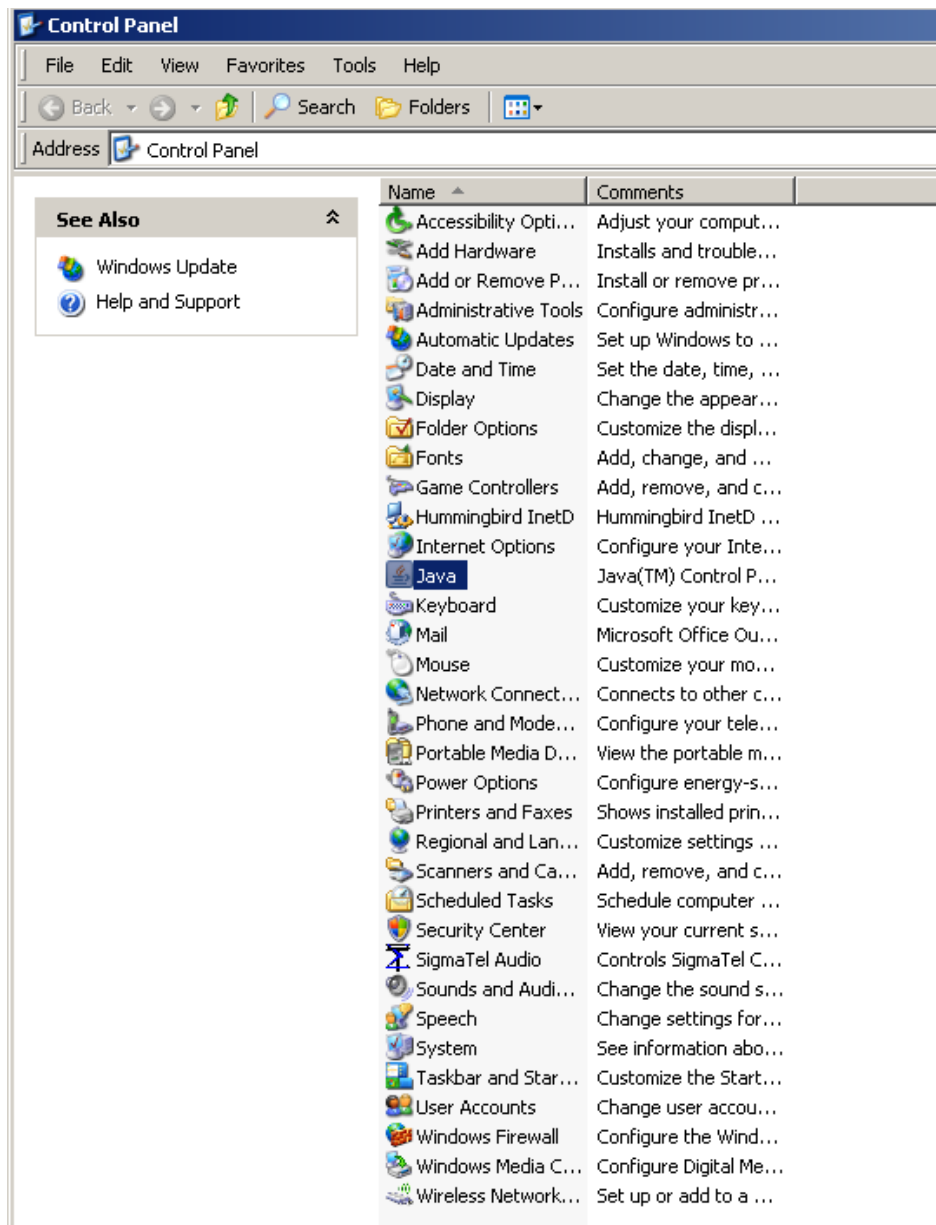
In the lower view you can select and deselect peak areas when you move the cursor inside the peak area you want to select and click the right mouse button the popup will appear. With the “Determine Area” you select a peak like it is chosen in ASAPRatio. With “Determine Area (Col)” the new peak finding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

### 7.7.1 Chromatogram 3D viewer:

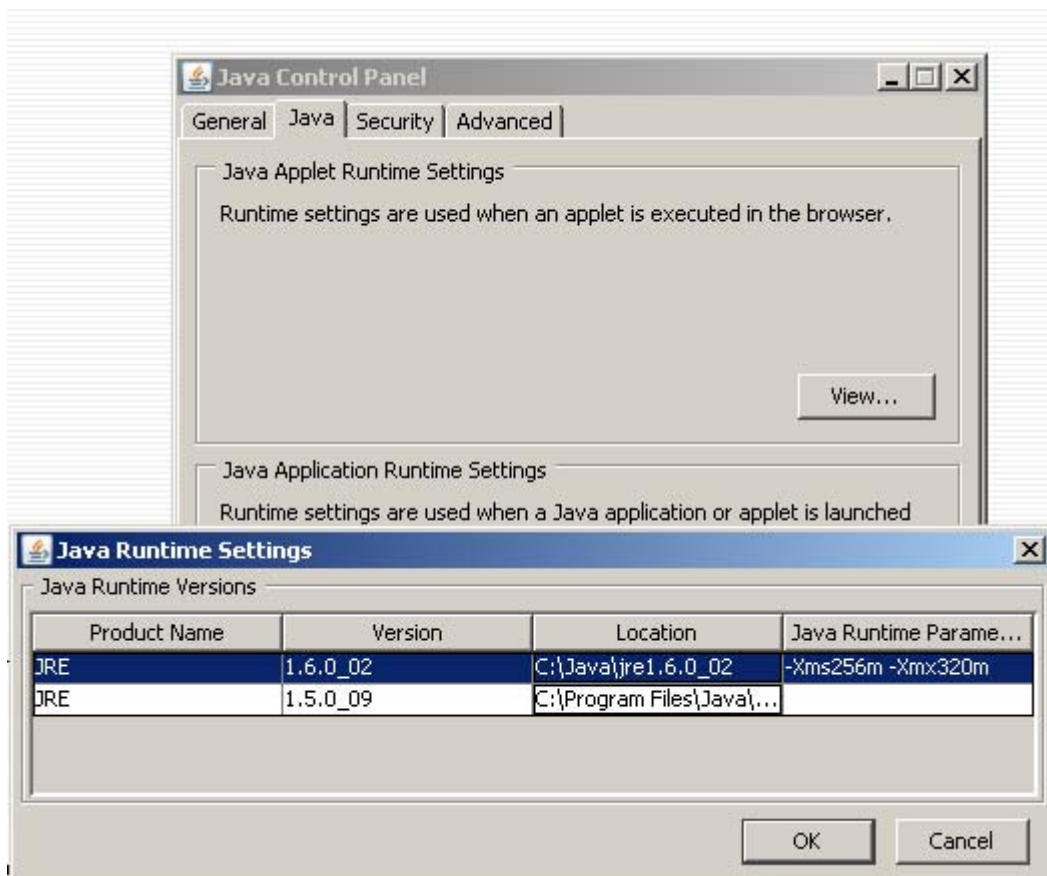
To run the 3D-viewer Java3D must be installed. You can download this from:

<http://java.sun.com/products/java-media/3D/download.html>

When you installed Java3D you have to reserve more memory for the applet. In Windows you have to go to “Control Panel” and then double-click on Java.



Then the Java Control-Panel opens:



Click on the Java tab and then in the Java Applet Runtime Settings on the “View” button. You should enter approximately the values I entered here (at least –Xmx320m should be used) and click on “OK”. Then it is necessary to restart your browser. Then in your browser it is possible to check your Java Console:

The browser window shows the Java Console with the following text:

```

Java Plug-in 1.6.0_02
Using JRE version 1.6.0_02 Java HotSpot(TM) Client VM
User home directory = C:\Documents and Settings\hartler

c: clear console window
f: finalize objects on finalization queue
g: garbage collect
h: display this help message
l: dump classloader list
m: print memory usage
o: trigger logging
p: reload proxy configuration
q: hide console
r: reload policy configuration
s: dump system and deployment properties
t: dump thread list
v: dump thread stack
x: clear classloader cache
0-5: set trace level to <n>

Memory: 260,224K Free: 240,529K (92%) ... completed.
  
```

The 'Tools' menu is open, showing 'Sun Java Console' as the selected option. Below the menu, the following sample IDs are listed:

```

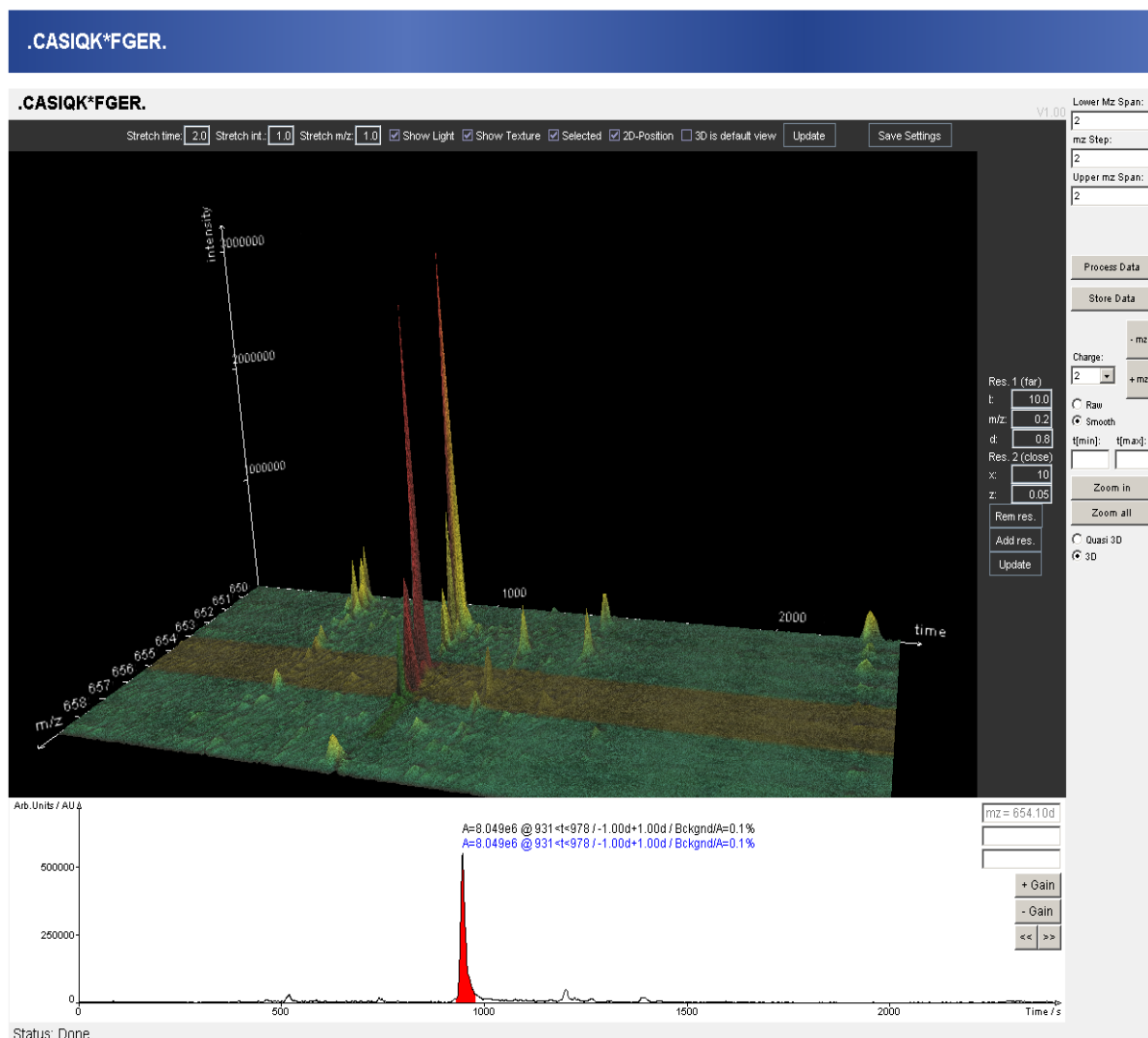
1=ICPL_Protmix_1lizu1he_B_
2=ICPL_Protmix_1lizu1he_A_
3=ICPL_Protmix_1lizu1he_C_
  
```

To the right of the sample IDs is a table with the following data:

	Sequence
<input checked="" type="checkbox"/>	1 .ALK*#
<input checked="" type="checkbox"/>	2 .ALK*#
<input checked="" type="checkbox"/>	3 .ALK*#
<input checked="" type="checkbox"/>	1 CASIC

When you click in the Java Console on “m” you can check the memory used. The option –Xms is the permanently reserved memory and the –Xmx is the maximum memory that could be used if needed. When you start the Java3D viewer (clicking on the radio button Java 3D) and you get java.lang.OutOfMemory you have to less memory to run the 3D applet.

Now to the 3D viewer:



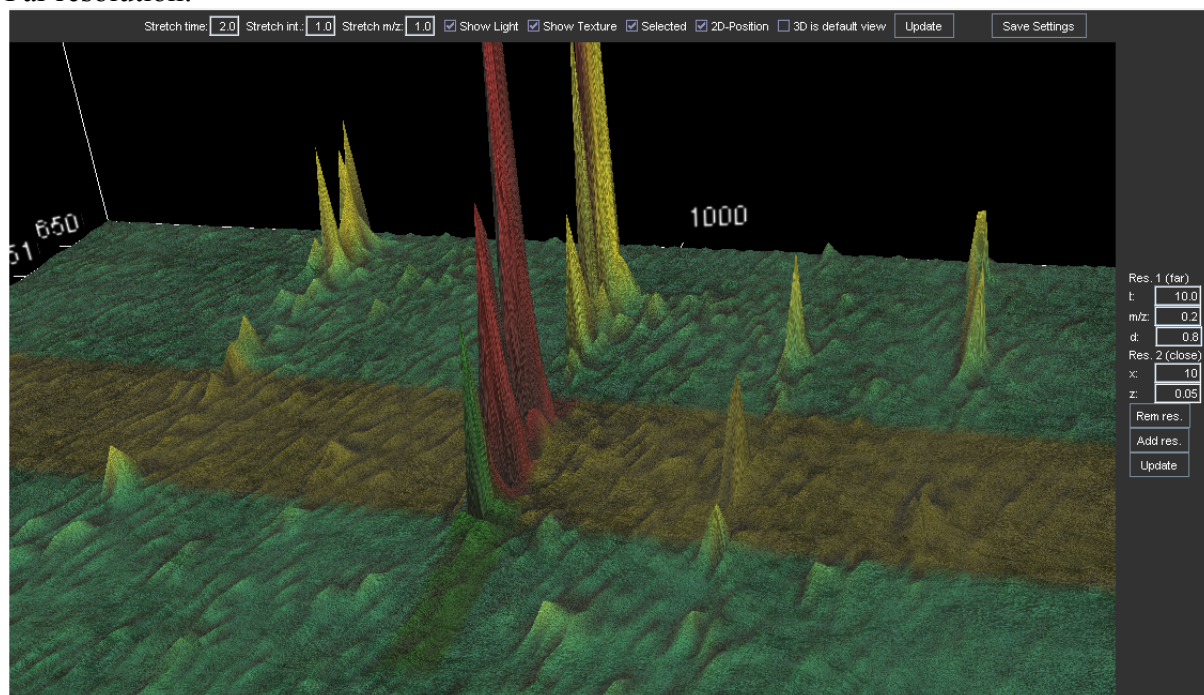
The memory used for this applet is mainly dependant on the resolution used and on effects like “Show Light” or “Show Texture”.

With the “Update” buttons you execute your changed settings.

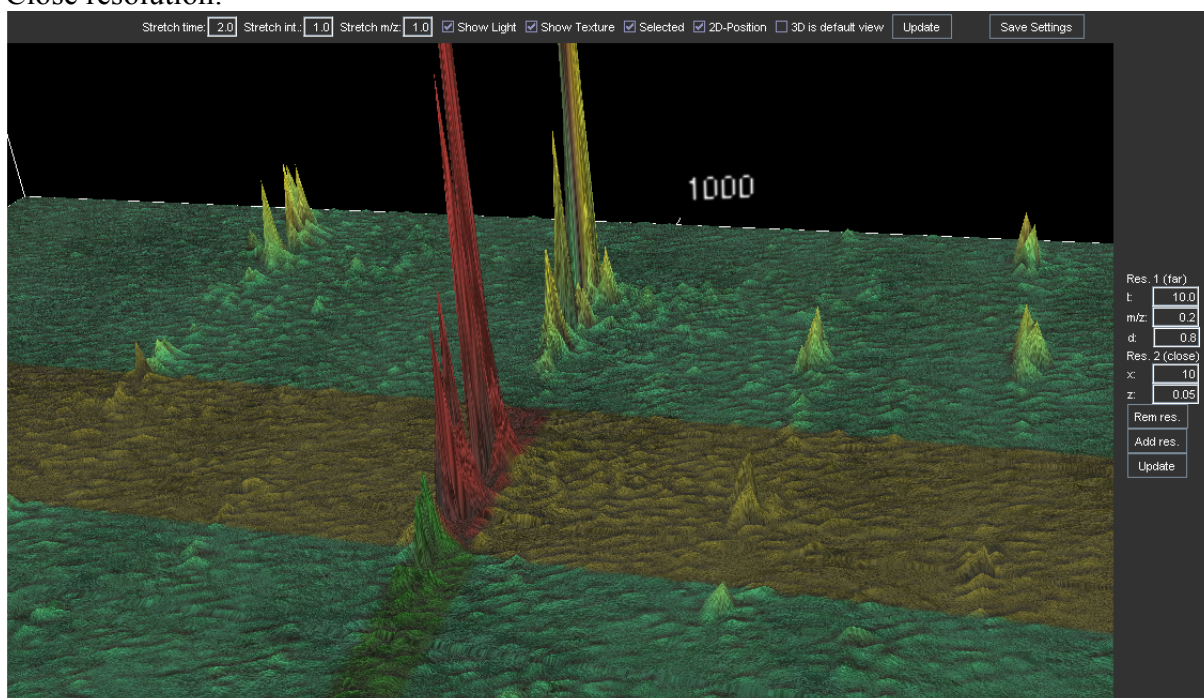
With “Stretch time” you can stretch or tighten the time coordinate. With “Stretch int.” you can stretch or tighten the intensity coordinate. With “Stretch m/z” you can stretch the m/z axis.

With show lights you can have light effects and with “Show Texture” the surface is covered with a texture. The light and texture option makes it easier to realize bumpiness on the surface. The “Selected” option shows the selected peaks in red and green. The “2D-Position” option shows the position of the 2D chromatogram displayed below in gold in the 3D chromatogram. On the right menu you can specify how the time and the m/z axis should be resolved. Here in this example I used two resolutions depending on the distance to the object. When you come nearer it will automatically switch to a higher resolution.

Far resolution:



Close resolution:



t: time in seconds which is used for one data point

m/z: m/z distance which is used for one data point

d: distance to the chromatogram object to switch to a higher resolution (has nothing to do with m/z or t).

The user can store for himself his own resolution settings and the rest of the settings described here with “Save Settings”. The “3D is default view” option has just an effect when you click afterwards on “Save settings”. When you checked this option, the next time you open a chromatogram viewer applet the 3D view will be used automatically.

Be careful with the resolution settings because they are causing the memory consumption of the applet. When you first visit the 3D view an automatic setting is calculated, which is adjusted to your data. When you once stored your own settings, these automatic settings will never be called again. So be careful when you first took a look at high resolution data (in a smaller range) and switch then to low resolution data (in a broader range). The viewer will still use the high resolution settings (if you did not save different ones) and run out of memory. Once the Java Console runs out of Memory all the browser windows have to be closed and the browser must be restarted. Very often the Java Console is still causing problems. The best is, once a browser window is opened to open the Java Console before any page is visited (then I have never problems). For this applet I had the experience that the Firefox browser is better, since for the Firefox more memory can be allocated for applets than the IE.

## 7.8 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:

### Select two modifications

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

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*DGAGDVAFVK.	2	128293.22	661789.1	0.19385816417949464	5.15841055357407
<input type="checkbox"/>	2	.CLK*DGAGDVAFVK.	2	195198.17	634894.9	0.30744957945007906	3.2525658411654166
<input type="checkbox"/>	3	.CLVEK*GDVAFVK.		0.0	0.0	NaN	NaN
<input checked="" type="checkbox"/>	2	.CLVEK*GDVAFVK.	2	1307267.75	1664997.8046875	0.7851468310166081	1.2736471198708146
<input checked="" type="checkbox"/>	1	.CLVEK*GDVAFVK.	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

