

MASPECTRAS 2.3

User Guide

In this user guide each 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.

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1. General Information

Bioinformatics Graz

Home | logout | User data | Password | Preferences | You are logged in as **Juergen Hartler**

MASPECTRAS
MAss SPECTrometry Analysis System

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This will be your first impression of MASPECTRAS.

The main view is divided into 3 sections:

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

1.1 The header section

Bioinformatics Graz


Home | login | logout | please login


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:

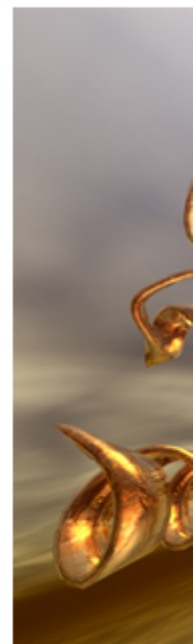


Welcome to MASPECTRAS

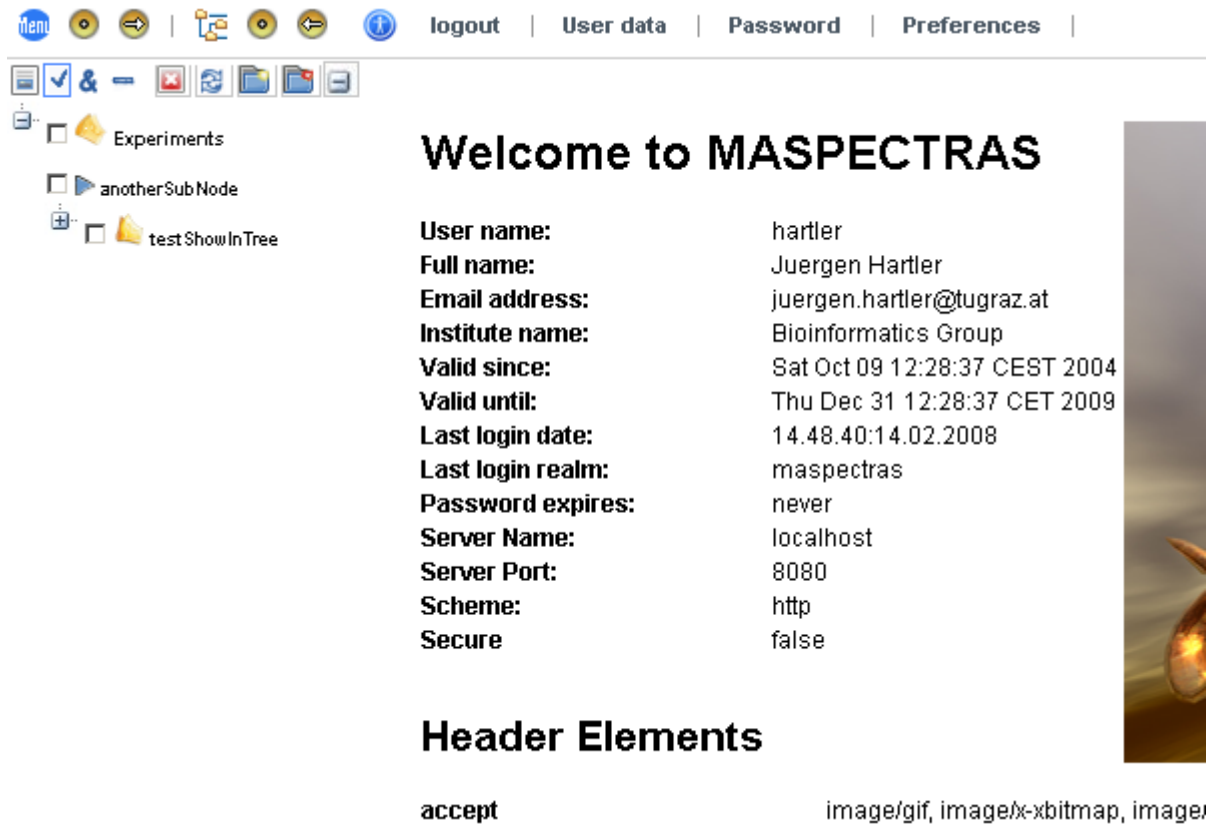
User name:	hartler
Full name:	Juergen Hartler
Email address:	juergen.hartler@tugraz.at
Institute name:	Bioinformatics Group
Valid since:	Sat Oct 09 12:28:37 CEST 2004
Valid until:	Thu Dec 31 12:28:37 CET 2009
Last login date:	14.48.40:14.02.2008
Last login realm:	maspectras
Password expires:	never
Server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



The screenshot displays the MASPECTRAS web interface. At the top, there is a menu bar with icons for 'menu', 'logout', 'User data', 'Password', and 'Preferences'. Below this, a tree menu on the left shows a hierarchy: 'Experiments' (with a folder icon), 'anotherSubNode' (with a folder icon), and 'test ShowInTree' (with a folder icon). The main content area is titled 'Welcome to MASPECTRAS' and displays user information in a table-like format:

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

Below the user information, the text 'Header Elements' is displayed. At the bottom, there is a line of code: `accept image/gif, image/x-xbitmap, image/`.

- : this shows a menu bar in a new window:

Home

logout | User data | Password | Preferences

Welcome to MASPECTRAS

User name: hartler
Full name: Juergen Hartler
Email address:
Institute name:
Valid since:
Valid until:
Last login date:
Last login realm:
Password expires:
Server Name:
Server Port:
Scheme: Secure

http://localhost:8080 - ...

Sample Generation

Experiment

Sample

Sampleorigin

Organism

Taggingprocess

Sample Processing

Mass Spectrometry

MS-Analysis

Management

2004
2009

Header E

accept
referer
accept-language
content-type
accept-encoding
user-agent
host
content-length
connection
cache-control
cookie

map, image/jpeg, image/pjpeg, application/msword, */*
aspectras/jsps/login.jsp
m-urlencoded
e; MSIE 6.0; Windows NT 5.1; SV1; .NET C
ement=7EBmT9CkBhU=:4vdbu8wEX8cC
42A162C439F45329BF4665680F

: 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:

logout | User data | Password | Preferences






You are logged in as **Juergen Hartler**

gives the possibility to:

- Log out
- Show detailed information about your user account
- Change your password
- Displays your user
- 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"/>
<input type="button" value="Save"/>	

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 )

107 Proteins found

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

Proteins per page:
 [15]
25
50
100

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 theyensis 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

107 Proteins found

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

Proteins per page:
 [15]
25
50
100

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

The information that will be displayed on the screen is customizable to the needs of the end-user. The user can select the information by clicking on the checkboxes and update the view on the data by pressing the button “Update”.

“Save Settings” allows the user to store his own display settings. Whenever the user enters the same page his settings will be displayed by default.

1.2.3 Scrolling bar


Proteins per page: **[15]** 25 50 100
 107 Proteins found << Previous | Page 2 of 8 | Next >> go to page go

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

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

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

1.2.4 Select input Fields

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 2.6 “Dictionary”.

1.2.5 Multiple input Fields and other buttons

Detection Agents: ?

Detection Agent: detectAgent + ○ X

Detection Agent: + ○ X

Add detection agent

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

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

Rehydration solutions: ?

Rehydration solution: myGelSubstance + ○

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 X. When the + button is next to an image the image is displayed at the bottom of the page.

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


? Rehydration solution X

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

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:

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 

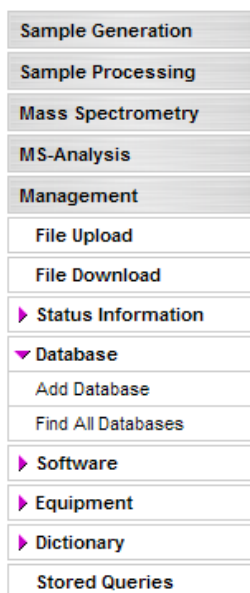


: unselects all of the previously select items and collapses all nodes of the tree

2. Management Section

2.1 Database

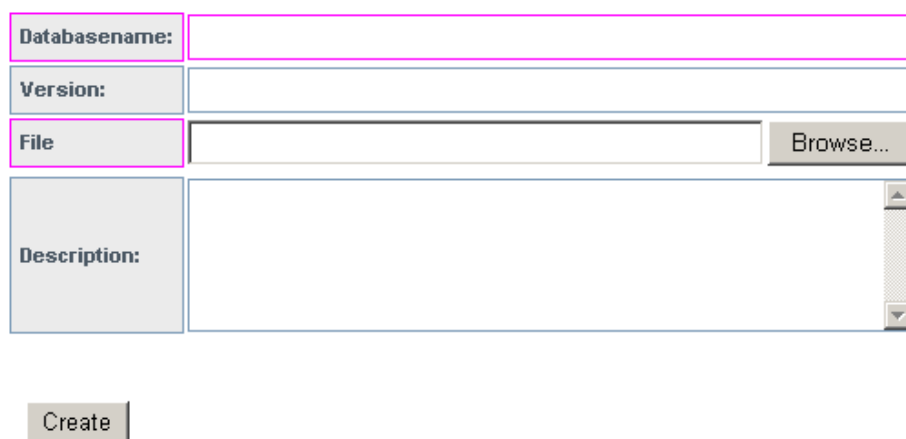
By clicking Management-> Database in the menu-bar you reach the general Database Section. MASPECTRAS needs the original sequence databases to find out the corresponding protein sequence.



A vertical menu with the following items: Sample Generation, Sample Processing, Mass Spectrometry, MS-Analysis, Management (highlighted), File Upload, File Download, Status Information (with a right-pointing arrow), Database (with a downward-pointing arrow), Add Database, Find All Databases, Software (with a right-pointing arrow), Equipment (with a right-pointing arrow), Dictionary (with a right-pointing arrow), and Stored Queries.

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.

New Database



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 followed by a 'Browse...' button.
- 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:	(gi\ vd+)\
Rule to parse description string from Fasta file:	[^]* (.*)
Rule to parse organism from Fasta file:	[^]*([^\w\s]+)\ .*
URL to the public database to retrieve information:	http://eutils.ncbi.nlm.nih.gov/entrez/eutils/efetch.fcgi?db=protein&ret
Parser for the URL information:	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 is for the information page. By default parsers are provided for IPI, Uniprot and GenBank (Since less annotations are directly available, the GenBank parser delivers not so much information as the IPI parser). If you want to enhance the existing parsers or write your own parser please visit 2.1.1.

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]Ogi|172
MRSYSNPENGGQINDNINYSKRPTMLPENLSLSNYDMDSFLGQFFSDNNMQLPHSTYEQHLQGEQQNPTNPNYFPPEFD
ENKVDWKQEKPKPAPSFADNNSFDNVNSSKLTNPSPVQPNIVKSESEPAANSKQNEVVEATSVEKAKENVAHESGTPESG
GSTSAPKSKKQRLTADQLAYLLREFSKDTPPPAIREKIGRELNIPERSVTIWFQNRRAKSKLISRRQEEERQRIILREQR
ELDSLNLQKVSQAFADHEVLSTSPYVGGIAANRQYANTLLPKPTRKTGNFYMKSGPMQSSMEPCIAESDIPRQSLSSST
YYNSLSFNAVPSVSSQRKYSASSYSAIPNAMSVSNAQAFDVESPPSSYATPLTGIRMPQFESDLYSYPREVSPSSGGYRMFG
HSKPSSYKASGPFVREPMMATGHRMRTSSEPTSYDSEFFYFSCITLLVIGLWKRLRASPDLMCFYSPPKKLFAYLIQFQGIQ
YRIEYSFFVIESIHVFRVEEPLLNELSATASSRDKPAPNEYWLQMDIQLSVPPVFHMITSEGQGNCTDFTEGNQASEVLL
HSLMGRATSMFQMLDRVRASPELGSVIRLQKGLNPHQFLDPQWANQLPRQPDSSVFDHQGRNPFIQGLSHDTSSEYGNK
SQFKRLRSTSTPARQDLAQHLLPDKTNTTEGLMHAQSVSPITQAMKSANVLEGSSTRLNSYEPSVSSAYPHHNLAALNDNT
QFGLGTSNISYPLSAPSDVGLPRASNSPSRPVMPHNTQGINTKIDMAAQFPNSQTGGTLPNSWSMNTNVSVPFTTQN
REFGGIGSSSISTMTNAPSQQLSQVFPFGDVSLATENSVPYSGFEVPSESVYAQARTNSSSVSAGVAPRLFIQTPIPLAS
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]
MPFSFLAQFPFPCKSISSHSLGVNSPGRGSHGNLNVFWYKLSISGLIEEDIVVDSPGFVVISLLLWLVEVGLDILVLFPPV
AFVPGFATVVIPIPLKLENVFLGDIWFVVDVGLDSSDVLSIVFIPL
```

```
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; Adel6p [Saccharomyces cerevisiae]
MGKYTKTAILSVYDKTGLLDLAKGLVENNVRIASGGTANMVREAGFPVDDVSITHAPEMLGGRVKTLLHPAVHAGILAR
NLEGDEKDLKEQHIDKVDVFCVNLVYFKETVAKIGVTVQEAVEEIDIGVTLRLAAAKNHSRVTLSDPNDYSIFLQDLS
KDGEISQDLNRNRFALKAFEHTADYDAAISDFFRKQYSEGKQALPLRYGCNPHQRPAQAYITQEEELPFKVLGCTPGYINL
LDALNSWPLVKELASLNLPAASFKHVSFAGAAVGLPLSDVERQVYFVNDMEDLSPLACAYARARGADRMSSFGDFIAL
SNIVDVATAKIIISKEVSDGVIAPGYEPEALNLSKKKNGKYCILQIDPNYVPGQMESREVFVTLQQRNDIAINQSTFK
EIVSKNKALTEQAVIDLTVATILVLKYTQSNVSVYAKNGMVVGLGAGQQSRIHCTRLAGDKTDNWWLRQHPKVLNMMKWAG
IKRADKSNAILDLFTVGRIEGPEKVDYESKFEEVPEPFTKEERLEWLSKLNNVSLSSDAFFFPDPNVYRAVQSGVKFITA
PSGSVMDKVVFAADSFDIVYVENPIRLFHH
```

```
Rule accession_rule: gi|6323056,gi|1709914,gi|7433574,gi|1480728,gi|2204263,
Rule description_rule: AICAR transformylase/IMP cyclohydrolase; Adel6p [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 the 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, then this rule didn’t return anything (this 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.

2.1.1 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, Uniprot and GenBank (here all of the information not available) and therefore there are the `IPIParser.jar`, `UniprotFlatfileParser.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 . 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 (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

Sample Generation
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► Status Information
► Database
► Software
► Equipment
► Dictionary
Stored Queries

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_1lizu1he_A_c1	rawdata	2008-02-13				
2	252	ICPL_Protmix_1lizu1he_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

File

Local File

File Type

Comment

Upload

☐

Raw-File

MS-Parameters

SpectrumMill

SpectrumMill Before Version A.03.02

SM Config

SM Custom Config

Mascot

Sequest

XITandem

Omssa

Omssa Modification File

Phenyx

TPP-pepXML

TPP-protXML

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

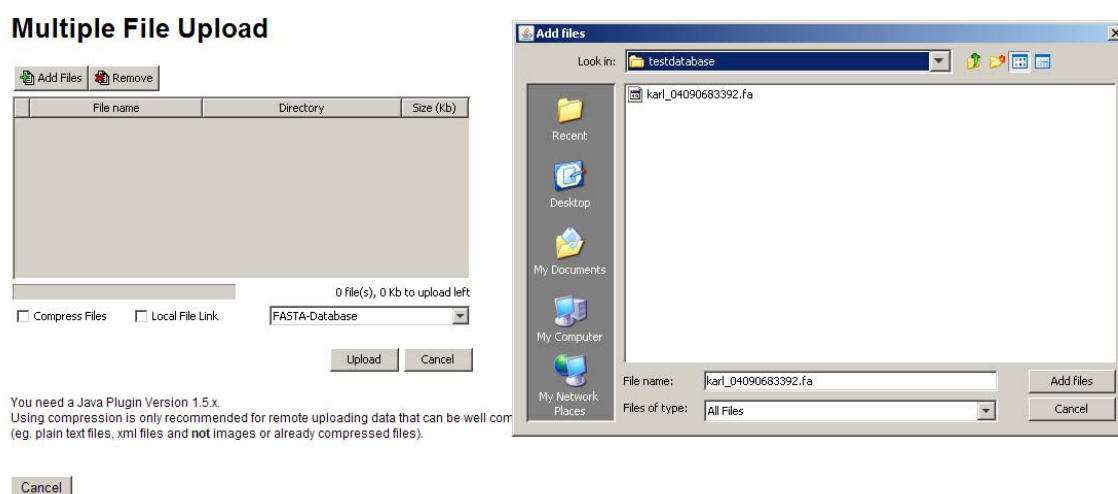
Gel2D Warping Map

LC-Column Parameters

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. For Phenyx, you must rename your pidres.xml file to a name that reflects your sample (e.g. S123P15.xml), the reason is that just one file with the same name can be stored. 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.

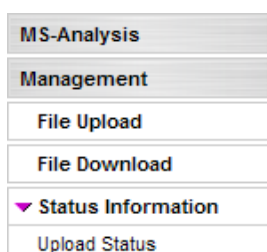
When you click “New multiple file upload” you come to the multiple file upload applet:



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.



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 File Download

Sample Generation
Sample Processing
Mass Spectrometry
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File Upload
File Download
► Status Information
► Database
► Software
► Equipment
► Dictionary
Stored Queries

By clicking Management -> File Download you reach the download section where all of the exported files from MASPECTRAS are listed:

5 FileDownloads found

Page 1 of 1

FileDownloads per page: 15 [25] 50 100 200

go to page go

Nr.	Name				
1	human erythroid leukemia cells 1021+1022				
2	human erythroid leukemia cells 1023+1024				
3	chronic phase patient 516+517				
4	accelerated phase patient 1 507+508				
5	accelerated phase patient 1 513+514				

FileDownloads per page: 15 [25] 50 100 200

5 FileDownloads found

Page 1 of 1

go to page go

2.5 Software




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

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

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

2.6 Dictionary

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

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

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

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

New MaspectrasDictionary

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

Create

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

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

43 MaspectrasDictionarys found

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

go to page [go](#)

Nr.	Domain	Value	Description		
1	MsResolutionlimit	10% valley			✗
2	MsResolutionlimit	FWHM			✗
3	esiSypplyType	static			✗
4	esiSypplyType	fed			✗
5	esiSolventFlowrateUnits	microlitres/min			✗
6	esiSolventFlowrateUnits	microlitres/min			✗
7	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			✗

2.7 Equipment





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

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

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"/>






















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

2.8 Stored Queries

Sample Generation
Sample Processing
Mass Spectrometry
MS-Analysis
Management
File Upload
File Download
► Status Information
► Database
► Software
► Equipment
► Dictionary
Stored Queries

By clicking Management -> Stored Queries you reach the download section where all of the stored queries from MASPECTRAS are listed and can be edited:

StoredQuerySet

 Query  Edit Display Settings

4 StoredQuerySets found | Page 1 of 1 | StoredQuerySets per page: 15 [25] 50 100 200 go to page go

Nr.	QueryName			
1	third-add-test12			
2	first-add-test			
3	sec-add-test			
4	dfasf1			

4 StoredQuerySets found | Page 1 of 1 | StoredQuerySets per page: 15 [25] 50 100 200 go to page go

3. Sample Description

3.1 Experiment

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

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

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

New Experiment

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

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>

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 <input type="text"/> 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 <input type="text"/> 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 ExperimentCreate Sample for ExperimentAdd SamplesCompare 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:	<input type="text"/> 
Add Sampleorigin	

Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="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		Samples per page: 15 [25] 50 100	
2 Samples found	Page 1 of 1	2 Samples found	Page 1 of 1
go to page <input type="text"/> go		go to page <input type="text"/> go	

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

> >

< <

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

Samples per page: 15 [25] 50 100		Samples per page: 15 [25] 50 100	
2 Samples found	Page 1 of 1	2 Samples found	Page 1 of 1
go to page <input type="text"/> go		go to page <input type="text"/> 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 (7).























3.3 Sampleorigin

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

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

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

New Sampleorigin

Name:	<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"/>
<div>Create</div>	

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

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

Sampleorigin

 Query
 Edit Display Settings

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

Nr.	Name	Organism			
1	aGoodOrigin	Human			

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

3.4 Organism

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

Sample Generation

▶ Experiment

▶ Sample

▶ Sampleorigin

▼ Organism

Add Organism

Find All Organisms

▶ Taggingprocess

Mass Spectrometry

MS-Analysis

Management

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

New Organism

SpeciesName:

TaxonomyId:

StrainIdentifier:

RelevantGenotype:

Owned by User:

☐

Owned by Inst.:

☒

Bioinformatics Group

Create

The species name and taxonomy-id can be exported to PRIDE see 7.1.

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

Organism

Query
 Edit Display Settings

1 Organisms found

Page 1 of 1

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

Nr.	SpeciesName			
1	Human			

1 Organisms found

Page 1 of 1

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

3.5 Taggingprocess

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

Sample Generation

▶ Experiment
 ▶ Sample
 ▶ Sampleorigin
 ▶ Organism
 ▼ Taggingprocess
 Add Taggingprocess
 Find All Taggingprocesses

Mass Spectrometry

MS-Analysis

Management

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

New Taggingprocess

Name:

LysisBuffer:

TagType:

TagPurity:

ProteinConcentration:

TagConcentration:

FinalVolume:

IncubationTime:

Owned by User:

☐

Owned by Inst.:

☒

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					

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

If you have entered values like the following:

Tree View

refresh tree

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

Sample quantification April 2006

Edit Display
Settings

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								

Other analyte 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:

37

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
Treated Analyte myTreatedSample
 Edit Display Settings

refresh tree

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

Gel 1D

add Gel 1D

Gel 2D

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

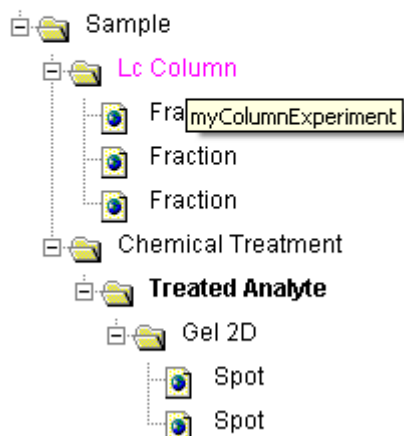
There are 5 different processing methods. A Gel1D leads to bands (for detailed information see chapter 4.2 Gel1D), a Gel2D leads to spots (for detailed information see chapter 4.3 Gel2D), a LC-Column leads to Fractions (for detailed information see chapter 4.4 LC-Column), a Chemical Treatment leads to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

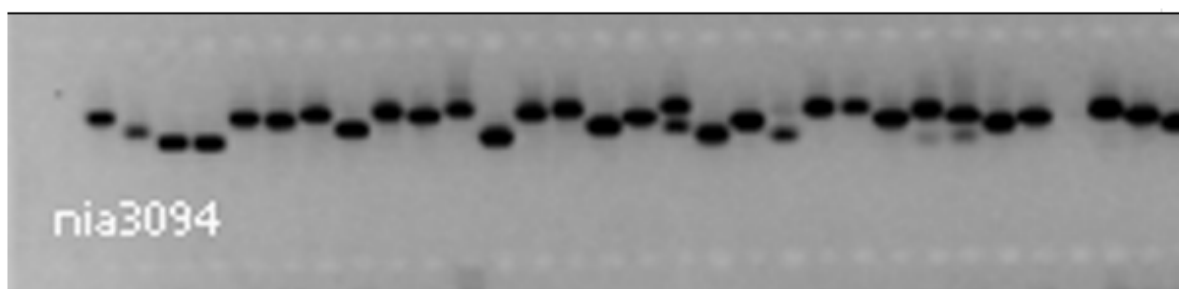
For the “Acquisition Component” you can select the whole selected “Gelmatrix” named with “Main” (you will find this select field, when you click on the “Gel” tab) or one of the components of the “Gelmatrix”. The references to the files (mostly images) which you can select in the “Image” tab, must be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

Edit Gel2D

Edit Display Settings

Gel2dd: test1t1

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

The screenshot shows the 'Buffer' tab in the 'Gel' software. The 'Buffer X' section is active, displaying 'BufferProtocolY' in a text area. Below this, the 'Running Buffers:' section lists two buffers: 'anotherBuffer' and 'testAdding'. Each buffer entry has a green plus icon and a blue circle icon, and a red 'X' icon.

New Spot

Title:	testASpot			
Area:	1.5			?
Intensity:	2.0			?
LocalBackground:	3.0			?
Annotation:	Annotation			?
AnnotationSource:	AnnotationSource			?
Volume:	4.0			?
Normalisation:	anotherOne			?
NormalisedVolume:	5.5			?
ApparentMass:	6.0			?
ApparentPi:	7.0			?
Description:	Description			?
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

Other analyte Processing Steps
add Other Analyte Processing Step

Chemical Treatment Processing Steps
add Chemical Treatment Processing Step

Massspec Experiments
add/remove Massspec experiments

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

Lc Columns								
Nr.	Title	Description	InternalLength	InternalDiameter	FlowRate	InjectionVolume		
1	myColumnExperiment							

add Lc Column

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

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

LC Column

Run Phases

Run Settings

Detection

Mobile phase components

Mobile phase component:

myFirstComponent1

1.0

Mobile phase component:

mySecondComponent2

2.0

Add mobile phase component

Gradient step 1:

Gradient Type:

constant

12.0

[min]

Purpose:

aGoodPurpose

Composition

Component:

mySecondComponent2

2.0

Add component

Type:

calibration and washing

Substance:

oneMoreTEstWithOneCompon

Time

1.0

Volume

2.0

Add between run

Gradient step 2:

Gradient Type:

gradient

12.0

[min]

Purpose:

asdfasdf

Composition

Component:

mySecondComponent2

3.0

4.0

Component:

myFirstComponent1

12.0

14.0

Add component

Add between run

Add gradient step

Update

add Fraction



Nr.	FractionId	StartPoint	EndPoint	ProteinAssay		
1	fasfafd	1.0	2.0	3.0		

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

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

Edit Fraction

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

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

Update

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

4.5 Chemical Treatment

Sample testSample

 Edit Display Settings

Gel 1D

add Gel 1D

Gel 2D

add Gel 2D

Lc Columns

add Lc Column

Other analyte Processing Steps

add Other Analyte Processing Step

Chemical Treatment Processing Steps

add Chemical Treatment Processing Step

Massspec Experiments

add/remove Massspec experiments

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

Chemical Treatment Processing Steps

Nr.	Digestion	Derivatisations		
1	trypsinDigestion			

[add Chemical Treatment Processing Step](#)


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

Show Chemicaltreatment

 [Edit Display Settings](#)

Digestion:	<input type="text" value="trypsinDigestion"/>
Derivatisations:	<input type="text"/>

[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:	<input type="text"/>
---------------------	----------------------

[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

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

> >

< <

Massspecexperiments per page: 15 [25] 50 100

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

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

Massspecexperiments per page: 15 [25] 50 100

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

Return

Adding massspec experiments to an analyte works the same way as adding samples to experiments (see chapter 3.2.2). The only difference is that only those mass spectrometry experiments are displayed on the left side, which are not already added to an analyte, while

the sample can be added to several experiments. For detailed information how to create mass spectrometry experiments see 6.1 “Mass spectrometry experiment”.

4.8 Gel Substance

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

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

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

New GelSubstance

Gelsubstanceld:

Component 1

✗

Name:

Concentration:

[mmol]

Component 2

✗

Name:

Concentration:

[mmol]

Add a component

Create

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

GelSubstance

 Query
 Edit Display Settings

6 GelSubstances found
Page 1 of 1
GelSubstances per page: 15 [25] 50 100

go to page go

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

6 GelSubstances found
Page 1 of 1
GelSubstances per page: 15 [25] 50 100

go to page go

4.9 Gel Matrix

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

Sample Generation

Sample Processing

▶ GelSubstance

▼ Gelmatrix

Add Gelmatrix

Find All Gelmatrices

▶ Buffer

▶ Detectionagent

▶ Reagent

Mass Spectrometry

MS-Analysis

Management

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

New Gelmatrix

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

Add a component

Create

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

Gelmatrixs per page: 15 [25] 50 100

4 Gelmatrixs found

Page 1 of 1

go to page go

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

Gelmatrixs per page: 15 [25] 50 100

4 Gelmatrixs found

Page 1 of 1

go to page go

4.10 Buffer

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

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

With the “Add Buffer” you can add buffers.

New Buffer

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

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

Buffer

Query Edit Display Settings

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

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

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.

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

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

New Detectionagent

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

Add antibody

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

5. Mass Spectrometry


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





5.1 Mass Spectrometry Machine

The main part of this section is the mass spectrometry and the other parts (except “Controlsoftware” see chapter 5.5 “Control Software”) are linked to this part. There are two ways how to reach this part. The first one is by the link in the create/edit page of the mass spectrometry experiment (see chapter 6.1 “Mass spectrometry experiment”), the second one is by clicking on Mass Spectrometry->Massspecmachine.

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

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

New Massspecmachine 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"/> 
Add mass-analyzer	
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="Bioinformatics Group"/>

Create

If your desired ionsource or mz-analysis 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 ionsources in chapter 5.2 “Ionsource” and about mz analysis in chapter 5.3 “Mzanalysis”. With the link “Add mass-analyzer” you can add additional mass analyzers. The link “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 Massspecmachines” button you get an overview of all your mass spectrometry machines:

Massspecmachine

 Query
 Edit Display Settings

Massspecmachines per page: 15 25 50 100

1 Massspecmachines found
Page 1 of 1
go to page go

Nr.	Name	ModelName			
1	myMassspecmachine	myModel			

Massspecmachines per page: 15 25 50 100

1 Massspecmachines 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

▶ Massspecmachine

▶ 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](#)

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

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

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

5.2.1 Electrospray

New IonSource

Name:	myTestIonSource		
Type:	ESI		
Supply			
SupplyType:	fed		
CycleTime MS1:		[ms]	✗
Add Cycle Time			
Solvent			
SolventComposition:			
SolventFlowrate:			
SolventFlowrateUnits:			
Interface			
InterfaceManufacturer:			
InterfaceName:			
InterfaceCatalognumber:			
InterfaceDescription:			
Sprayer			
SprayTipManufacturer:			
SprayerName:			
SprayerCatalognumber:			
SprayerCoating:			
SprayerDescription:			
SprayTipVoltage:		[V]	
SprayTipDiameter:			
ConeVoltage:		[V]	
Acceleration and Dissociation			
Accelerationvoltage MS1:		[V]	✗
Add Accelerationvoltage			
InSourceDissociation:	false		
NebulisingGas:			
NebulisingGasPressure:		[bar]	

Create

When you change the type to “ESI”, you get the electro spray input form. When you change the “SupplyType” to “fed” then the link “Add Cycle Time” appears and you can enter cycle times for all your MS-levels. In the section “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:	<input type="text"/>		
Type:	MALDI <input type="button" value="v"/>		
Plate and Matrix			
PlateComposition:	<input type="text"/>	<input type="button" value="v"/>	<input type="button" value="x"/>
MatrixComposition:	<input type="text"/>	<input type="button" value="v"/>	<input type="button" value="x"/>
DepositionTechnique:	<input type="text"/>		
Voltage Settings			
GridVoltage:	<input type="text"/>	<input type="button" value="V"/>	
Add Accelerationvoltage			
Post Source Decay			
PsdType:	<input type="text"/>	<input type="button" value="v"/>	
PsdDescription:	<input type="text"/>		
ExtractionDelayed:	false	<input type="button" value="v"/>	
Laser Settings			
LaserType:	<input type="text"/>	<input type="button" value="v"/>	
LaserWavelength:	<input type="text"/>	<input type="button" value="nm"/>	
LaserPower:	<input type="text"/>	<input type="button" value="microJ"/>	
FocusDiameter:	<input type="text"/>	<input type="button" value="microm"/>	
AttenuationDetails:	<input type="text"/>		
PulseDuration:	<input type="text"/>	<input type="button" value="ns"/>	
ShotFrequency:	<input type="text"/>	<input type="button" value="Hz"/>	
AvgNrOfShotsFiredOnSpectrum:	<input type="text"/>		
Owned by User:	<input type="checkbox"/>		
Owned by Inst.:	<input checked="" type="checkbox"/>	Bioinformatics Group <input type="button" value="v"/>	
<input type="button" value="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:	<div>Description</div>
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.

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

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

New Mzanalysis



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

If your desired 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 detection in chapter 5.4 “Detection”.

There are 9 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 5.3.8 and other 5.3.9) available and the input page changes correspondingly.
















With a click on the button “Find All Mzanalysis” you get an overview of all your mz analysis apparati:

Mzanalysis

 Query
  Edit Display Settings

Mzanalysis per page: 15 [25] 50 100

4 Mzanalysis found
 Page 1 of 1
 go to page go


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

Mzanalysis per page: 15 [25] 50 100

4 Mzanalysis found
 Page 1 of 1
 go to page go

5.3.1 Ion optic

New Mzanalysis

Name:	<input type="text"/>
Detection:	<input type="text"/> 
Type:	<input type="text" value="Ion Optic"/>
Description:	<input type="text"/>
Collisioncell:	<input type="checkbox"/>
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Bioinformatics Group"/>

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 5.3.10).

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:			
Detection:			
Type:	TOF		
ReflectronState:			
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 5.3.10).

5.3.5 Ion Trap

New Mzanalysis

Name:			
Type:	Ion Trap		
GasType:			
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 Linear Trap

Same input page like ion trap see 5.3.5.

5.3.7 Orbitrap

Same input page like ion trap see 5.3.5.

5.3.8 FT-ICR

Same input page like ion trap see 5.3.5.

5.3.9 Other

Same input page like ion optic see 5.3.1.

5.3.10 Collision Cell

New Mzanalysis

Name:	<input type="text"/>		
Detection:	<input type="text"/>	<input type="button" value="v"/>	<input type="button" value="v"/>
Type:	<input type="text" value="other"/>		
Description:	<input type="text"/>		
Collisioncell:	<input checked="" type="checkbox"/>		
GasType:	<input type="text"/>	<input type="button" value="v"/>	<input type="button" value="v"/>
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.

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



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

New Detection

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

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

Detection












 Query  Edit Display Settings

Detections per page: 15 [25] 50 100

3 Detections found

Page 1 of 1

go to page go

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

Detections per page: 15 [25] 50 100

3 Detections found

Page 1 of 1

go to page go




5.5 Control Software

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

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

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



New Controlsoftware

PackageName:	<input type="text"/>
IsolationWidth:	<input type="text"/>
Criteria	
Criteria:	<input type="text"/> 
Add Criteria	
Softwares	
Software:	<input type="text"/>  
Add Software	
Owned by User:	<input type="checkbox"/>
Owned by Inst.:	<input checked="" type="checkbox"/> <input type="text" value="Bioinformatics Group"/>
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 2.5 “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.

New MassspecexperimentEdit Display Settings

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

Create

If the desired mass spectrometry machine is not in the select box you can click the blue button on the right side of the select box and you will reach the create page of the mass spectrometry machine (see chapter 5.1 “Mass Spectrometry Machine”). If the desired control and analysis software is not in the select box, click the blue button on the right side of the select box and

you will reach the create page of the control software (see chapter 5.5 “Control Software”). To select a raw File click the blue button next to the “Raw File” input field. The following page will appear:

File Upload

 Query
 Edit Display Settings

Selected File:

Clean selection
Accept Selection

13 Files found
Page 1 of 1

Files per page: 15 25 50 100
 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

13 Files found
Page 1 of 1

Files per page: 15 25 50 100
 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_1hzu1l	Sample: test
Mascot1hzu1l	Sample: test
060606FTc2_phosphb_bsa_1hzu1lSequest	Sample: test
060606FTc2_phosphb_bsa_1hzu1lSpectrMill	Sample: test
bsa_1hzu1lXTandem	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 Δ means the allowed threshold difference between the first and the rest of the found hits for one search. For Phenyx, there is a threshold for the peptide- and the protein score. 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: 2.0 +3: 2.5	Δ :	1.0
Peptide Prophet Threshold:	0.0	Δ :	1.0
Mascot Peptide Threshold:	+1: 15.0 +2: 20.0 +3: 20.0	Δ :	100.0
SpectrumMill Peptide Threshold:	10.0	Δ :	100.0
SpectrumMill Config File			
SpectrumMill User Config File			
XTandem Peptide Threshold:	30.0	Δ :	1000
Omssa e-Value Threshold:	20.0	Δ :	1000
Omssa Modification File:			
Phenyx Thresholds:	Protein: 10.0 Peptide: 5.0		
Protein Prophet Threshold:	0.9		
Min Peptide Length:	5		
# Peptides for protein:	1		
Alignment:	NONE		
Just top intensity peaks:	<input type="checkbox"/>		
Quantification tolerance +/- m/z [Da]:	<input checked="" type="checkbox"/> 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

> >

< <


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_1hzu1ISequest	sequest
<input type="checkbox"/> bsa_1hzu1IXTandem	xtandem
<input type="checkbox"/> 060606FTc2_phosphb_bsa_1hzu1IOMSSA	omssa
<input type="checkbox"/> Mascot1hzu1I	mascot
<input type="checkbox"/> 060606FTc2_phosphb_bsa_1hzu1ISpectrumMill.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:	2.0	+3:	2.5	Δ:	1.0
Peptide Prophet Threshold:	0.0				Δ:	1.0		
Mascot Peptide Threshold:	+1:	15.0	+2:	20.0	+3:	20.0	Δ:	100.0
SpectrumMill Peptide Threshold:	10.0				Δ:	100.0		
SpectrumMill Config File	<input type="text"/>							
SpectrumMill User Config File	<input type="text"/>							
XITandem Peptide Threshold:	30.0				Δ:	1000		
Omssa e-Value Threshold:	20.0				Δ:	1000		
Omssa Modification File:	<input type="text"/>							
Phenyl Thresholds:	Protein:	10.0	Peptide:	5.0				
Protein Prophet Threshold:	0.9							
Min Peptide Length:	5							
# Peptides for protein:	1							
Alignment:	NONE							
Just top intensity peaks:	<input type="checkbox"/>							
Quantification tolerance +/- m/z [Da]:	<input checked="" type="checkbox"/> 1.0							

×

Quant Method: ASAPR Standard

Affected AAs: DE Var: ☐ Mass shift:

1. Partner Time shift: Mass shift: 3.18 ✗

2. Partner Time shift: 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 2.3):

“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 three 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. Tree view (see section 1.3)
3. To use the

Compare Results

button.

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

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

Searches

Query Edit Display Settings Quant-Settings

For Re-Quantification:

Quantification tolerance +/-m/z [Da]: 1.0

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

Accept


All


None

Return

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. Furthermore MASPECTRAS detects automatically ontology for the modification by the mass shift. At this page it is possible change the modification number for fixed and variable modifications. To check the ontology you could use the “Ontology Lookup Service” of the EBI: <http://www.ebi.ac.uk/ontology-lookup/>

Nitrogen	14.003074	
Oxygen	15.994915	
Electron	5.49E-4	
C-term	17.00274	
N-term	1.007825	
Oxidation (XM)	15.994919	MOD:00425
NeutralLoss1	0.0	
ICPL_heavy (K)	111.04184	MOD:00789
NeutralLoss2	0.0	
ICPL_light (K)	105.021439	MOD:00790
NeutralLoss3	0.0	




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









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

1 = 060606FTc2_phosphb_bsa_1hzu1lSequest (Partitioning )
2 = Mascot1hzu1l (Partitioning )
3 = 060606FTc2_phosphb_bsa_1hzu1lSpectrMill.zip (Partitioning )

Proteins per page: 15 [25] 50 100 200

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



Nr.	Search	AccNr	GeneName	%SeqMax 	Score	# Prots	# Peps 	# Spec 		
1	1 2 3	gi 231300; 231300	Glycogen Phosphorylase b (E.C.2.4.1	54.81	2840.53	1	61	962		Kalign
2	1 2 3	162648; gi 162648	albumin [Bos taurus]; Gene_Symbol=a	39.87	1289.28	2	27	360		Kalign
3	2 3	gi 3318722; 3318722	Chain E, Leech-Derived Trypsin Inh	8.08	108.42	1	2	17		Kalign
4	1 2 3	gi 999627; 999627	Chain B, Porcine E-Trypsin (E.C.3.4	21.96	108.42	2	2	20		Kalign
5	1 2 3	39794653; gi 39794653	Keratin 1 [Homo sapiens]; Keratin 1	2.18	81.04	2	1	2		Kalign

Proteins per page: 15 [25] 50 100 200

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


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

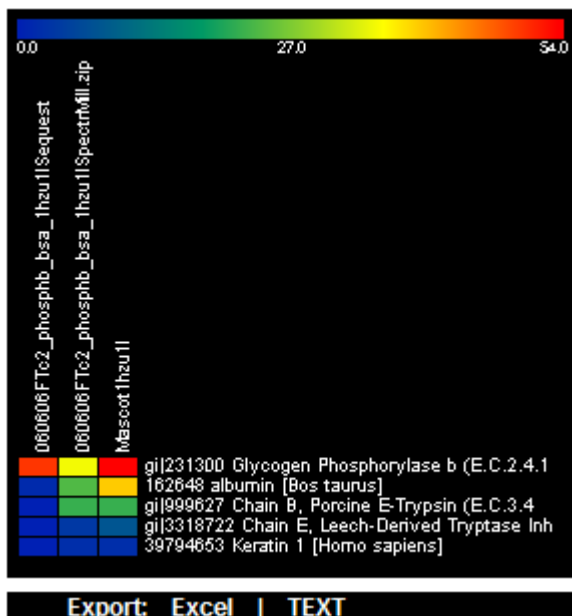
To Protein View >>

To Peptide View >>

Return


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. You can get a quick overview about the proteins found in the different searches, samples or experiments in a heat map with the  icon. The heat map can be generated for the sequence coverage, the number of proteins and the number of spectra (here a heat map of the sequence coverage in percent is shown).






When you reach the page the proteins are clustered. The proteins are sorted by their amount of found peptides. In a clustered group the protein with the most found peptides is displayed as anchor. If some proteins have the same amount of peptides the one with SwissProt

annotations is favoured, if several have SwissProt annotations the shortest protein is used as anchor. 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  button you get all proteins of that cluster listed.

Protein

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

1 = 060606FTc2_phosphb_bsa_1hzu1ISequest (Partitioning )
2 = Mascot1hzu1I (Partitioning )
3 = 060606FTc2_phosphb_bsa_1hzu1ISpectMill.zip (Partitioning )

Proteins per page: 15 [25] 50 100 200
5 Proteins found | Page 1 of 1 | go to page go

Nr.	Search	AccNr	GeneName	%SeqMax	Score	# Prots	# Peps	# Spec		
1	1 2 3	gi 231300; 231300	Glycogen Phosphorylase b (E.C.2.4.1	54.81	2840.53	1	61	962		Kalign
2	1 2 3	162648; gi 162648	albumin [Bos taurus]; Gene_Symbol=a	39.87	1289.28	2	27	360		Kalign


Details from




Nr.	Search	AccNr	GeneName	%SeqMax	Score	# Peps	# Spec
1	1 2 3	gi 162648; 162648	Gene_Symbol=albumin [Bos taurus] \	39.71	1289.28	27	360
2	1 2 3	gi 418694; 418694	serum albumin precursor [validated]	38.06	1252.41	26	584

Sequence

gi-162648
gi-418694

LEGEND: Proteinsequence Gaps

Go to Multiple Sequence Alignments: Muscle TCOffee Expresso Get Fasta: 

3	2 3	gi 3318722; 3318722	Chain E, Leech-Derived Tryptase Inh	8.08	108.42	1	2	17		Kalign
4	1 2 3	gi 999627; 999627	Chain B, Pordine E-Trypsin (E.C.3.4	21.96	108.42	2	2	20		Kalign
5	1 2 3	39794653; gi 39794653	Keratin 1 [Homo sapiens]; Keratin 1	2.18	81.04	2	1	2		Kalign

Proteins per page: 15 [25] 50 100 200
5 Proteins found | Page 1 of 1 | go to page go





Export Current View: Excel DOC TEXT PRIDE XML

The “Cluster Nr.” indicates the cluster where the protein is located. The order is the same as in the “Search” column.

If you don’t want to see the clustered view at all you can click on the “To Protein View>>” at the bottom of the page to get all proteins displayed.

Protein

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

1 = 060606FTc2_phosphb_bsa_1hzu1I (Partitioning )
2 = 060606FTc2_phosphb_bsa_1hzu1Iomssa (Partitioning )
3 = 060606FTc2_phosphb_bsa_1hzu1ISequest (Partitioning )
4 = 060606FTc2_phosphb_bsa_1hzu1IKTandem (Partitioning )

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

Nr.	Search	AccessionNum	Organism	GeneName	SequCovMax	Score	Cluster Nr.	Amount of Peptides
1	1 2 3 4	gi 231300	validated	Glycogen Phosphorylase b (E.C.2.4.1.1) (T State) Complex With AMP	53.97	51846.45	Cluster-4 Cluster-4 Cluster-3 Cluster-11	84
2	1 2 3 4	gi 418694	validated	serum albumin precursor [validated] - bovine	40.37	30102.72	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
3	1 2 4	gi 162648	Bos taurus	albumin [Bos taurus]	42.01	30183.17	Cluster-3 Cluster-3 Cluster-1 Cluster-7	40
4	4	gi 435476	Homo sapiens	cytokeratin 9 [Homo sapiens]	23.12	355.40	Cluster-1	9
5	4	gi 1346343	Homo sapiens	Keratin, type II cytoskeletal 1 (Cytokeratin 1) (K1) (CK 1) (67 kDa cyto keratin) (Hair alpha protein)	13.2	337.19	Cluster-2 Cluster-2 Cluster-4 Cluster-1	8
6	4	gi 39794653	Homo sapiens	Keratin 1 [Homo sapiens]	13.2	337.19	Cluster-2 Cluster-2 Cluster-1	8
7	4	gi 71528	human	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 massspecmachine analyzers and detectors and the controlsoftware. You can enter the global project-name (used in PRIDE to find data belonging to one another) in the “Edit Display Settings” at the input field “PRIDE project name:”. The results of the PRIDE-export can be downloaded in the “File Download” (see section 2.4).

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 coloured.


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

Furthermore, not just one query can be saved as default as described in 1.2.1, but here several queries can be saved by a given name. The name of the query-set can be changed or deleted in

the Stored Queries section described in 2.8; the selection can be made directly in the query box.

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

✕

☒ XK*: -6.03
 ☐ XM@: 15.99
 ☒ no mod

Lower Threshold 1:

Lower Threshold 2:

Amount of needed peptides:

Upper Threshold 1:

Upper Threshold 2:

☒ Normalize ☐ Remove incompletely modified


















p-Value Warning:

p-Value Threshold:

Accept
Save Settings
Remove Stored Settings

262 Proteins found
Page 1 of 11 [Next >>](#)

Proteins per page: [15](#) [25](#) [50](#) [100](#) [200](#)
 go to page [go](#)

Nr.	AccNr	*f0	Organism	GeneName	%SeqMax 	Score	# Prots	# Peps 	# Spec 		
1	spt P05736	1.03 p-V=0.000	Saccharomyces cerevisiae	60S ribosomal protein L2 (YL6) (L5)	62.85	835.72	3	15	59		Kalign
2	spt P14126	1.10 p-V=0.000	Saccharomyces cerevisiae	60S ribosomal protein L3 (YL1) (RP1)	44.56	631.51	3	14	41		Kalign
3	spt P40150	0.96 p-V=0.001	Saccharomyces cerevisiae	Heat shock protein SSB2	34.16	674.95	31	13	30		Kalign
4	emb CAA24631.1	1.01 p-V=0.000	Saccharomyces cerevisiae	pyruvate kinase	27.66	599.58	2	11	50		Kalign
5	spt P49626	0.95 p-V=0.014	Saccharomyces cerevisiae	60S ribosomal protein L4-B (L2B) (R)	44.88	607.00	6	10	44		Kalign
6	spt P40212	0.97 p-V=0.000	Saccharomyces cerevisiae	60S ribosomal protein L13-B	66.34	516.97	2	10	38		Kalign
7	spt P05735	1.193 p-V=0.449	Saccharomyces cerevisiae	60S ribosomal protein L19 (L23) (YL)	46.28	490.90	4	10	30		Kalign
8	spt P05753	1.26 p-V=1.000	Saccharomyces cerevisiae	40S ribosomal protein S4 (S7) (YS6)	48.85	385.53	2	9	17		Kalign
9	spt P23248	1.00 p-V=0.006	Saccharomyces cerevisiae	40S ribosomal protein S1-B (RP10B)	51.19	477.25	4	9	28		Kalign
10	rf NP_015194.1	0.89 p-V=0.001	Saccharomyces cerevisiae	Protein component of the large (60S)	43.44	367.97	4	9	25		Kalign
11	spt P41805	0.87 p-V=0.004	Saccharomyces cerevisiae	60S ribosomal protein L10 (L9) (Ubi)	49.78	494.76	2	9	31		Kalign
12	spt P26785	0.89 p-V=0.007	Saccharomyces cerevisiae	60S ribosomal protein L16-B (YL15)	49.75	335.69	6	9	19		Kalign
13	spt P05756	0.96 p-V=0.000	Saccharomyces cerevisiae	40S ribosomal protein S13 (S27A) (Y)	75.34	400.74	3	9	32		Kalign
14	spt P15108	1.02 p-V=0.000	Saccharomyces cerevisiae	ATP-dependent molecular chaperone H	17.19	531.64	12	9	34		Kalign

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

Refresh
Return

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

- : Download of the involved proteins in FASTA format

: Download of the alignment of the proteins

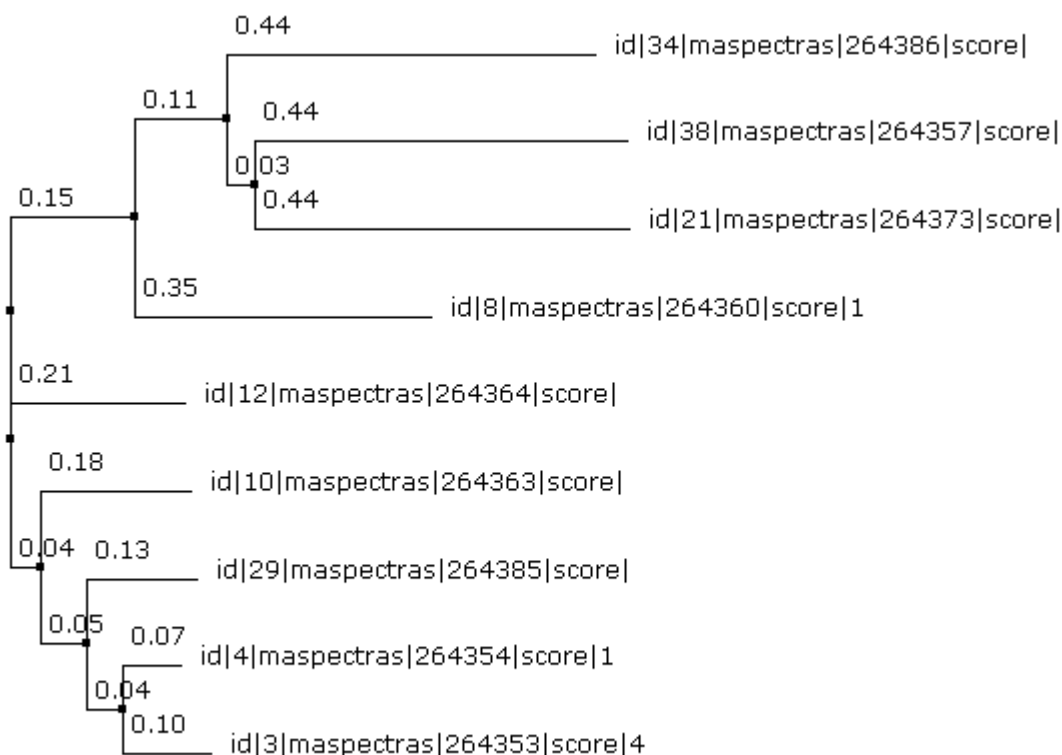
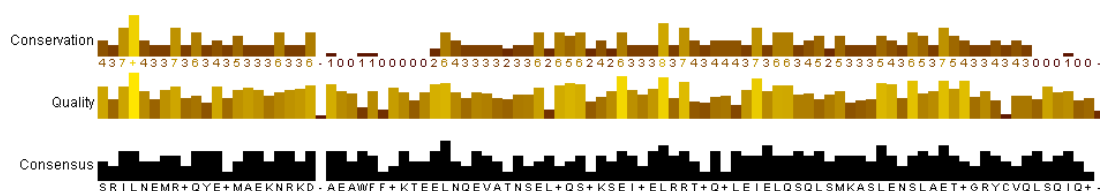
: Download the storage of the tree that you can see in Jalview at the end of this section

: The log-file of the alignment

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

: Starts Jalview applet to see the alignment

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 Q 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 Q 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 M R S D Y E A M V E K N R S D A E A W F T S K T D E L N Q E V A V H T K L Q T S K T E V T D L R R T L Q G L E I E L Q S Q L S M K A L E G T L A E T E A R Y G V Q L S Q I Q A .
 id|12|maspectras|264364|score|1-78: Q L L N N M R S D Y E Q L A E Q N R K D A E A W F N E K S K E L T T E I D N N I E Q I S S Y K S E I T E L R R N V Q A L E I E L Q S Q L A L K Q S L E A S L A E T E G R Y C V Q L S Q I H A .
 id|8|maspectras|264360|score|1-78: D S I I A E V M A D Y E E I A N R S R T E A E S W Y Q T K Y E E L Q Q T A G R H G D L R N T K H E I S E M N R M I Q R L R A E I D N V K K Q C A N L N A I A D A E Q G E L A L K D A R N .
 id|34|maspectras|264386|score|1-78: P A I I S S S N S N K N E N A V S T D T S T P A A A G A P E G K P P Q K T S N K K S L S S K E A I E E L K F S E K F K V P Y D I P K D M L E V L K R S S T L K S N S L P P K P I S K I .
 id|21|maspectras|264373|score|1-78: S V L L R L A E Y E A T L E E C C A K D D P H A C Y S T V F D K L K H L V D P Q N L I K Q N C D Q F E K L G E Y G F Q N A L I V R Y T R K V P Q V S T P T L V 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 F 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 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” (see 1.2.2). 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), based on mass spectrometry evidence, and/or on different GO-clusterings. Since the mass spectrometry evidence based clustering and the GO-based clusterings are calculated on the fly, pre-calculation of the alignment is not possible. Thus the fast alignment algorithm Kalign has been included.

The screenshot shows the MASPECTRAS Protein view. At the top, there's a header bar with "Protein" and navigation links: "Query", "Edit Display Settings", and "Quant-Settings". Below this, a status bar indicates "12 Proteins found" and "Page 1 of 1". A table lists 12 proteins with columns: Nr., AccNr, GeneName, Gene Symbol, Domains, %SeqMax, Score, # Prots, # Peps, # Spec, and a series of icons for various clustering methods (Kalign, Enz, Ens, Go, PblM, SPrt). A red circle highlights the "Kalign" icon for the first protein (KRT1). Below the table, a detailed view of the protein alignment is shown, with a URL bar indicating the file name and type. The alignment view includes a sequence viewer with amino acid sequences and a "Return" button.

Nr.	AccNr	GeneName	Gene Symbol	Domains	%SeqMax	Score	# Prots	# Peps	# Spec	Kalign	Enz	Ens	Go	PblM	SPrt
1	IPI00220327.3	KRT1 Keratin, type II cytoskeletal	KRT1		21.74	712.50	2	13	29						
2	IPI00009865.2	KRT10 Keratin, type I cytoskeletal	KRT10		18.89	398.10	44	8	14						
3	IPI00021304.1	KRT2 Keratin, type II cytoskeletal	KRT2		12.72	435.04	14	7	15						
4	IPI00019359.3	KRT9 Keratin, type I cytoskeletal 9	KRT9		17.02	361.38	1	6	8						
5	IPI00470657.1	~ Anti-colorectal carcinoma heavy c			18.35	385.64	1	6	79						
6	gi 136429	NS1 protein Influenza A/PR8 [NP_040			0.0	153.82	1	4	5						
7	gi 136429	Trypsin precursor			22.95	241.93	1	4	73						
8	IPI00383815.4	GFAP Isoform 2 of Glial fibrillary	GFAP		2.52	57.67	19	2	7						
9	IPI00387120.1	- Ig kappa chain V-IV region Len		IGv	7.9	23.34	5	1	1						
10	IPI00514599.5	SCNN1D Isoform 1 of Amiloride-sensi	SCNN1D		1.42	26.02	4	1	2						
11	IPI00829697.1	- Uncharacterized protein ENSP00000		IGv	9.41	85.72	1	1	1						
12	IPI00887164.1	LOC646057 similar to hCG2003024			4.34	61.84	2	1	12						

The procedure to display the alignment is similar to 7.2. First the “Load” button has to be clicked to start the alignment. On clicking the Java icon Jalview Alignment editor will be started to show the results.

Additional alignment methods are included with Muscle, TCOFFEE and Expresso. In order to use these alignment methods, you have to click the blue button to see the members of the group, and on the bottom of the newly opened box buttons for these clustering methods appear (see next figure).

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).

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

Add Clustering

Update | Display all | Display default Save Settings

Proteins per page: 15 [25] 50 100 200

90 Proteins found | Page 1 of 4 | Next >> go to page go

Nr.	AccNr	GeneName	%SeqMax	Score	# Prots	# Peps	# Spec		Kalign
1	IP100215790.6	RPL38 60S ribosomal protein L38	50.0	194.30	1	6	7		Kalign
2	IP100220362.5	Gene_Symbol=HSPE1 10 kDa heat shock	54.91	272.21	1	6	10		Kalign
3	IP100456429.3	Gene_Symbol=UBA52 ubiquitin and rib	41.41	285.92	2	6	29		Kalign

Details from

Nr.	AccNr	GeneName	%SeqMax	Score	# Prots	# Peps	# Spec		Kalign
1	IP100456429.3	Gene_Symbol=UBA52 ubiquitin and rib	41.41	285.92	34	6	29		Kalign
2	IP10020008.1	NEDD8 NEDD8 precursor	17.29	75.44	2	2	4		Kalign

Details from

Nr.	AccNr	GeneName	%SeqMax	Score	# Prots	# Peps	# Spec		Kalign
1	IP10020008.1	NEDD8 NEDD8 precursor	17.29	75.44	2	2	4		Kalign
2	IP100873768.1	NEDD8 Uncharacterized protein NEDD8	17.5	75.44	2	2	4		Kalign

Sequence

LEGEND: ProteinSequence Gaps

Go to Multiple Sequence Alignments: Muscle Tcoffee Expresso Get Fasta

Sequence

LEGEND: ProteinSequence Gaps

Go to Multiple Sequence Alignments: Muscle Tcoffee Expresso Get Fasta

Peptide Sequence

EGPRDQGR

ESTLHLVLR

IGDKGIPPDQGR

IPQIFVK

ITLEVPSTDIENVK

TLSDYNIQK

This example shows a protein list which is first clustered by the mass spectrometry evidence and then by the protein sequence. The third row has been expanded with the blue button and the content of the cluster (2 proteins) is shown (clustering by protein sequence). The protein at row two of the cluster is again the representative of a cluster (clustered by MS evidence) which is again expanded by the blue button. The remaining elements of a cluster or of the protein list will be continued after the extension of the cluster. 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”. The coloring of the peptides is the same like in the quick alignment view. The green arrow showing upwards has the purpose to change the anchor of a group. If you click on it the chosen element would stand on the top of a cluster-group.

Additionally, MASPECTRAS has the possibility to cluster the proteins according to GO-terms:

1. Clustering: Masspec Evidence 2. Clustering: GO-MolecularFunction

Add Clustering

Update | Display all | Display default Save Settings

Proteins per page: 15 [25] 50 100 200

68 Proteins found | Page 1 of 3 | Next >> go to page

Gene Ontology Graph of all Proteins:

Nr.	GeneOntology Term	P - Value	# Prots		
1	NONE	0.0	28		
2	copper chaperone activity	0.0010	2		

Details from

Nr.	AccNr	GeneName	%SeqMax	Score	# Prots	# Peps	# Spec		Kalign
1	IP100218144.3	COX17 Cytochrome c oxidase copper c	25.4	42.97	2	1	1		Kalign
2	IP100010863.5	ATOX1 Copper transport protein ATOX	13.24	20.91	1	1	1		Kalign

Gene Ontology in Java

GO Database Loaded: OBO

View Type: Tree Graph Child Depth: 1

Query GO id: GO:0016531 GO:0016531 Query

GO Graph:

```

graph TD
    A[GO:0016531] --> B[GO:000367]
    A --> C[GO:0005198]
    B --> D[GO:0005198]
    C --> D
    D --> E[GO:0043167]
    E --> F[GO:0043168]
    F --> G[GO:0046872]
    G --> H[GO:0046914]
    H --> I[GO:0005507]
    I --> J[GO:0016531]
  
```

Here the result view looks a little bit differently. As result GO-terms and not proteins are displayed, but if you click on the blue button you see the proteins that belong to this GO-term. The green button is for the display of the GO-graph. Comment: The GO-based clustering requires the fetch of external information (see 7.4), and for this the protein sequence database has to be configured correspondingly (see 2.1).

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 there 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
 ☒ Export Groups

☒ Hide Keratin
 ☐ Amount of Spectra
 ☐ PredictedMass
 ☐ Nr. of Proteins
 ☐ Quantification
 ☐ Show Decoy Statistics

Gene Ontology Information
☒ GO Term
 ☒ P-Value
 ☐ GO Id

List-size:

External links
☒ EntrezGene
 ☒ GO
 ☒ iHop
 ☒ UniprotSwissprot
 ☒ Vega
 ☒ Prosite
 ☒ Ensembl
 ☒ Pfam
 ☒ Kegg
 ☒ UniprotTrembl
 ☒ GeneCard
 ☒ RefSeq
 ☒ EnsemblHavana
 ☒ Pubmed
 ☒ Gen3D
 ☒ PathoSign
 ☒ InterPro

1. Clustering:

Add Clustering

Update | Display all | Display default

Save Settings

8 Proteins found

Proteins per page: 15 [25] 50 100 200

Page 1 of 1

go to page go

Nr.	AccNr	GeneName	# Peps	Enz	Ens	Hav	Go	Pfm	PbMd	iHop	Keg	G3D	SPrt	Trbl	PSgn	Vga	IPro	PrSt	RSq	GCd
1	IPI00470657.1	- Anti-colorectal carcinoma heavy c	7	Kalig	e!															
2	glj136429	Trypsin precursor	4	Kalig	e!															
3	gljapr8	NS1 protein Influenza A/PR8 [NP_040	4	Kalig	e!															
4	IPI00383815.4	GFAP Isoform 2 of Glial fibrillary	2	Kalig	e!															
5	IPI00387120.1	- Ig kappa chain V-IV region Len	1	Kalig	e!															
6	IPI00887164.1	LOC646057 similar to hCG2003024	1	Kalig	e!															
7	IPI00514599.5	SCNN1D Isoform 1 of Amiloride-sensi	1	Kalig	e!															
8	IPI00829697.1	- Uncharacterized protein ENSP00000	1	Kalig	e!															

8 Proteins found

Proteins per page: 15 [25] 50 100 200

Page 1 of 1

go to page go

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

89

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 X

MKWVTFISLLLLFSSAYSRGVFRDTHKSEIAHR**F****K****D****L****G****E****E****Q****F****K****G****L****V****L****I****A****F****S****Q****Y****L****Q****Q****C****P****F****D****E****H****V****K****L****V****N**
L**T****E****F****A****K****T****C****V****A****D****E****S****H****A****G****C****E****K****S****L****H****T****L****F****G****D****E****L****C****K****V****A****S****L****R****E****T****Y****G****D****M****A****D****C****C****E****K****Q****E****P****R****N****E****C****F****L****S****H****K****D****D****S****P****D****L****P****K****L**
K**P****D****P****N****T****L****C****D****E****F****K****A****D****E****K****K****F****W****G****K****Y****L****E****I****A****R****R****H****P****Y****F****A****P****E****L****L****Y****A****N****K****Y****N****G****V****F****Q****D****C****C****Q****A****E****D****K****G****A****C****L****L****P****K****I****E****T****M****R**
E**K****V****L****A****S****S****A****R****Q****R****L****R****C****A****S****I****Q****K****F****G****E****R****A****L****K****A****W****S****V****A****R****L****S****Q****K****F****P****K****A****E****F****V****E****T****K****L****V****T****D****L****T****K****V****H****K****E****C****C****H****G****D****L****L****E****C****A****D****D**
R**A****D****L****A****K****Y****I****C****D****N****Q****D****T****I****S****S****K****L****K****E****C****D****K****P****L****L****E****K****S****H****C****I****A****E****V****E****K****D****A****I****P****E****N****L****P****L****T****A****D****F****A****E****D****K****D****V****C****K****N****Y****Q****E****A****K****D****A****F**
L**G****S****F****L****Y****E****S****R****R****H****P****E****Y****A****V****S****V****L****L****R****L****A****K****E****Y****E****A****T****L****E****E****C****A****K****D****D****P****H****A****C****Y****S****T****V****F****D****K****L****K****H****L****V****D****E****P****Q****N****L****I****K****Q****N****C****D****Q****F****E**
K**L****G****E****Y****G****F****Q****N****A****L****I****V****R****Y****T****R****K****V****P****Q****V****S****T****P****T****L****V****E****V****S****R****S****L****G****K****V****G****T****R****C****C****T****K****P****E****S****E****R****M****P****C****T****E****D****Y****L****S****L****I****L****N****R****L****C****V****L****H****E****K**
T**P****V****S****E****K****V****T****K****C****T****E****S****L****V****N****R****R****P****C****F****S****A****L****T****P****D****E****T****Y****V****P****K****A****F****D****E****K****L****F****T****F****H****A****D****I****C****T****L****P****D****T****E****K****Q****I****K****Q****T****A****L****V****E****L****L****K****H****K**
P**K****A****T****E****E****Q****L****K****T****V****M****E****N****F****V****A****F****V****D****K****C****C****A****A****D****D****K****E****A****C****F****A****V****E****G****P****K****L****V****V****S****T****Q****T****A****L****A**

☐ 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](#)


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










The gene-name is displayed at the page head. The button opens the box with the protein sequence again, if you have closed it. Below the page head the searches are listed again. This time dyed in order to recognize them in the protein sequence. Underneath the possible combinations of the searches are colour-encoded as well.

The “Sequence” box has a little checkbox “All found in Red”, which shows all found parts of the sequence in red, if one colour is not easily visible.

Then the searches are listed again and the fixed modifications are given. At the end of the searches the variable modifications are indicated in one row. The affected amino acids are shown followed by the substitute for the modification in the peptide list and the mass shift after the colon.

Below the searches the found peptides are listed, sorted by the score. To indicate by which search the peptide has been found the numbers in the search column are denoted (the same way like in 7.1). If this sequence is a first hit, the sequence is in bold letters. When you uncheck the checkbox in front of a peptide, this peptide will be removed as found in the “Sequence” box. At the upper right part of the peptides listed there is the link “Compare Ratios of 2 Modifications”. Here you can compare the quantitative ratios of differentially labelled proteins (e.g. ICPL-light to ICPL-heavy), or all found peptides which carry a modification versus ones that do not carry the modification (see 7.8).

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@NOD@TISSK.@		
<input checked="" type="checkbox"/>	1	45.04	.YICD*NOD*TISSK.*		
<input checked="" type="checkbox"/>	1	26.62	.YICDNOD@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									X
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									X
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							×
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.	.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 by these queries, which takes a little bit longer processing time:

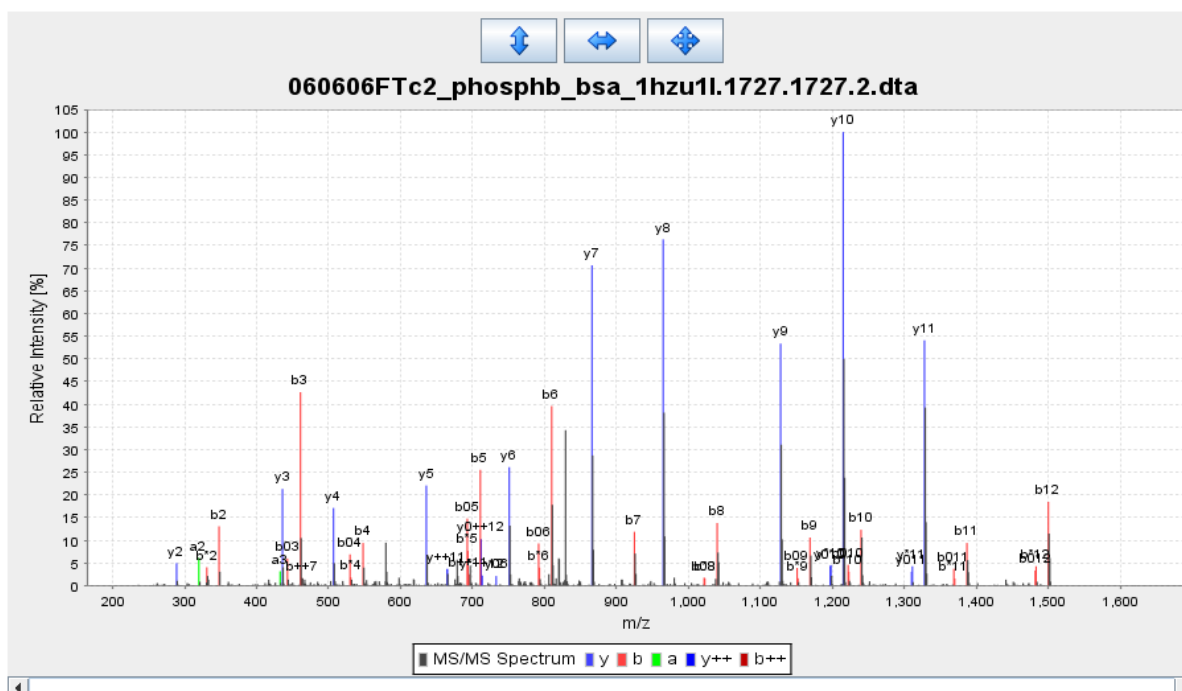
- **NrOfPassingSpectra:** a specific amount of spectra must be found for one peptide hit in one search
- **NrOfPassingFirstHitSpectra:** a specific amount of spectra must be found for one peptide hit in one search
- **NrOfTotalPassingSpectra:** a specific amount of spectra must be found for one peptide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

7.6 Spectrum View

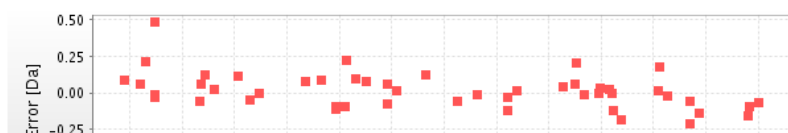
060606FTc2_phosphb_bsa_1hzu1l.1727.1727.2.dta

Edit Display Settings

K@LLSYVDDEAFIR



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

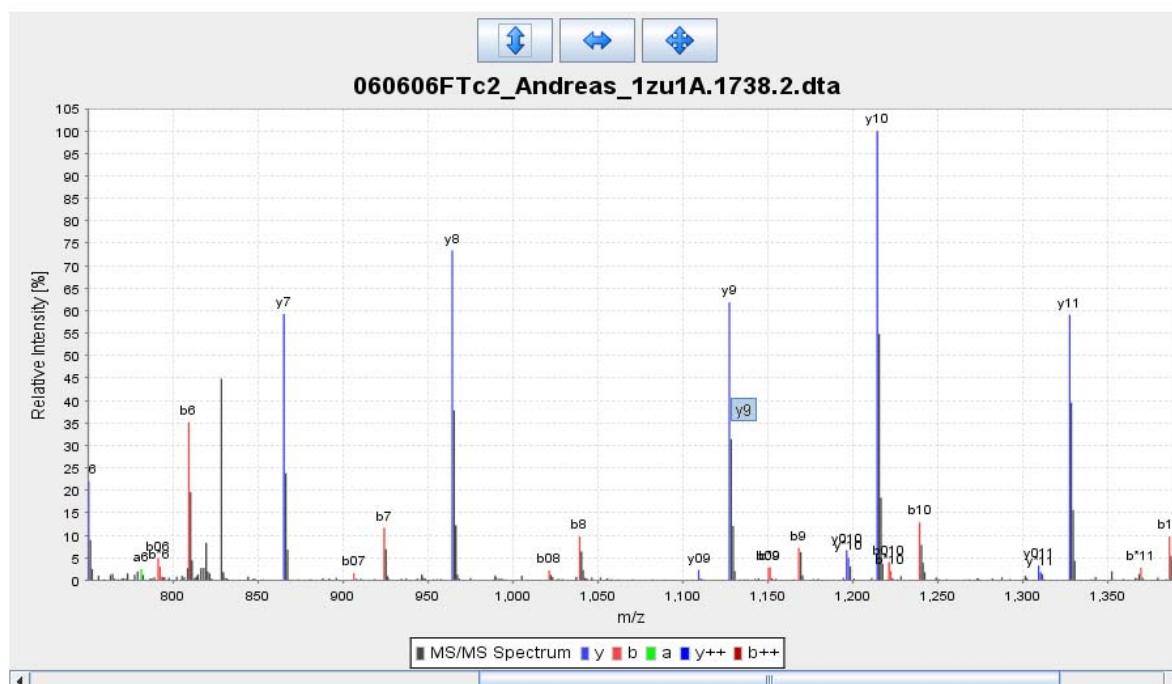


With “Edit Display Settings” you can select the series you want to be displayed. You can save your own display settings like in all the other pages.

With the select box below the “Edit Display Settings” box you can switch between the found hits.

Then there is a Java Applet with the spectrum (see 7.6.1) 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

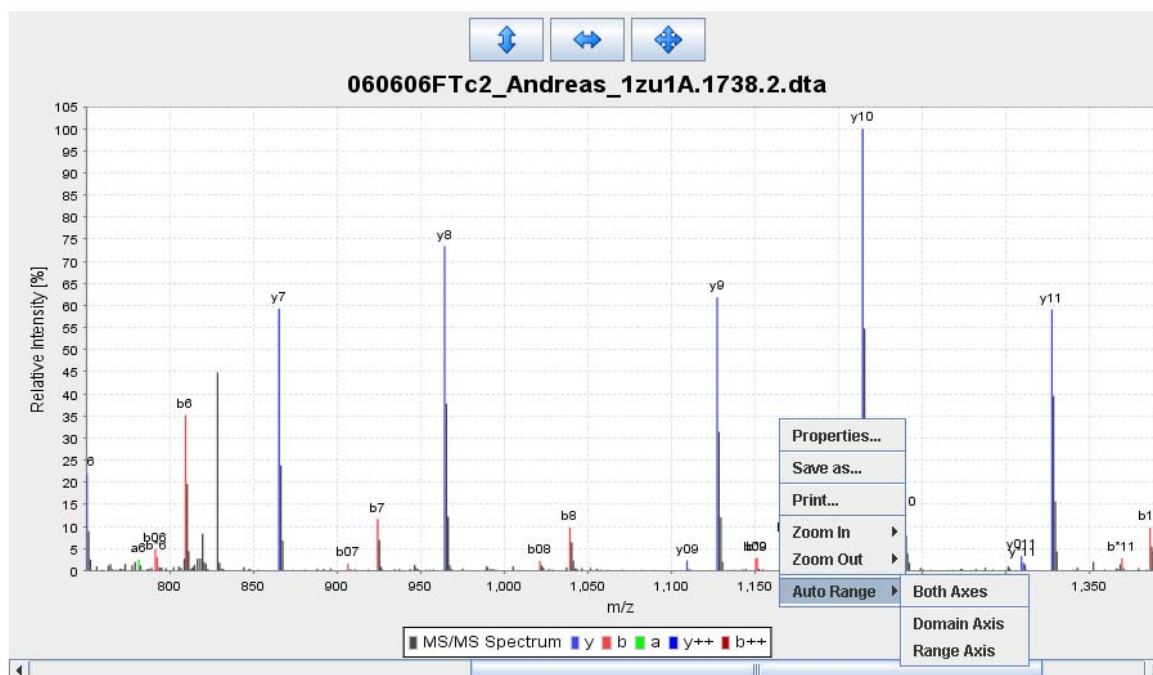


: zooms out the x-axis

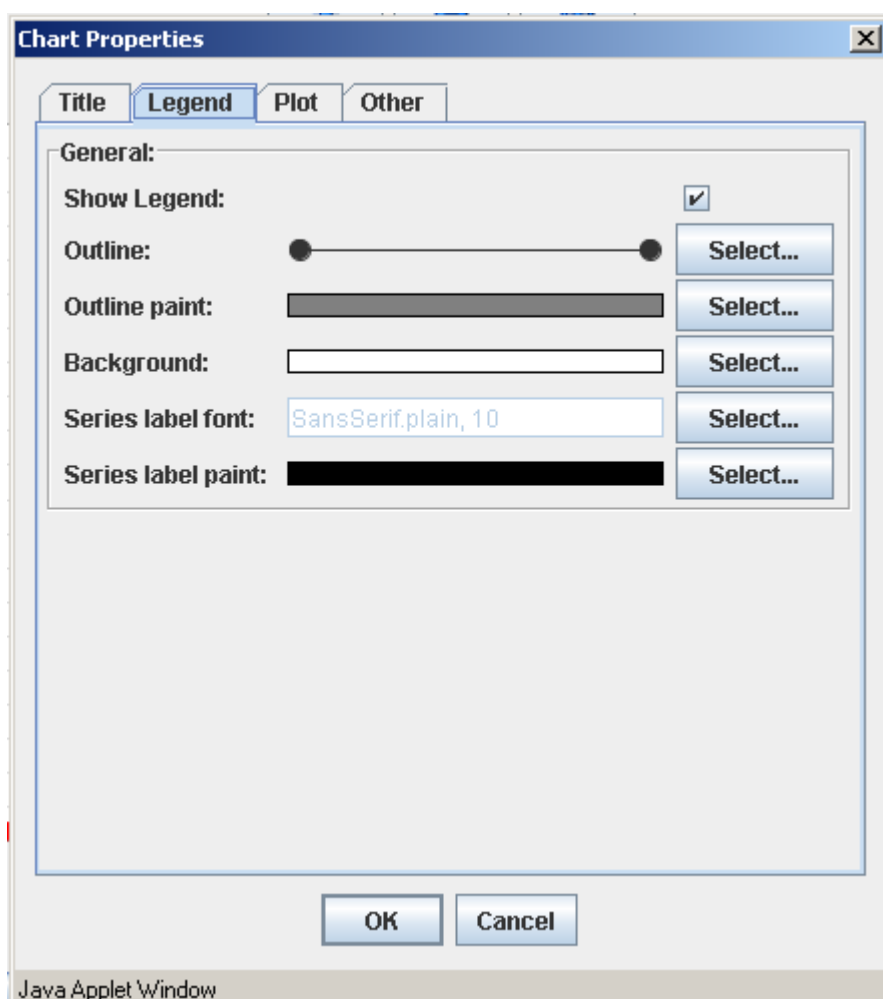


: zooms out both axes

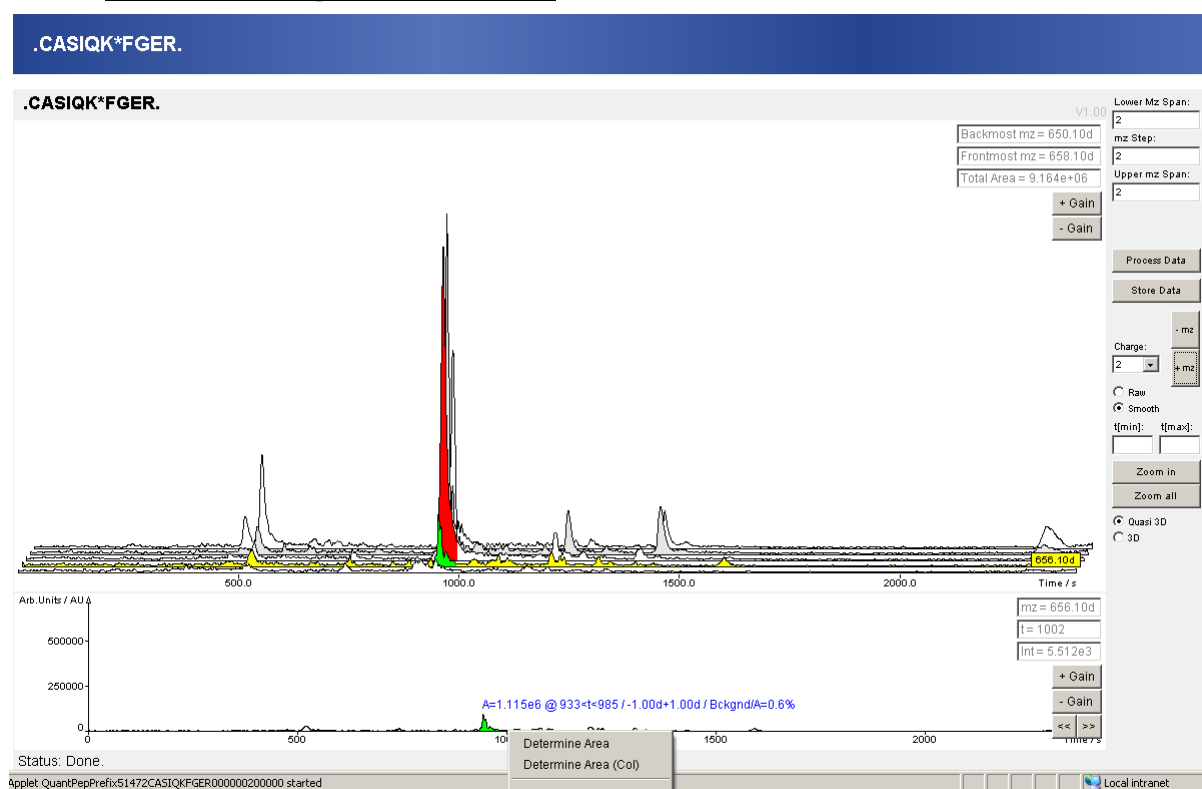
When you first click on the spectrum and then click with the right mouse button you will get a popup window where you have additional features:



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.

Backmost mz = 651.70d
Frontmost mz = 656.50d
Total Area = 8.964e+06
+ Gain
- Gain

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

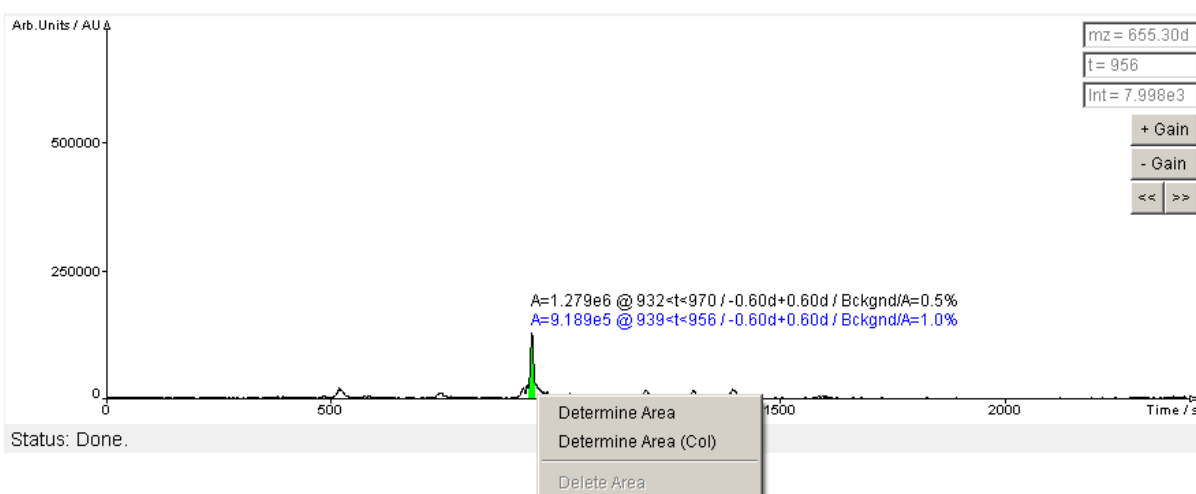
In the menu on the right side you can determine how many chromatograms you want to see in positive/negative m/z direction with “Upper mz Span”/”Lower Mz Span”. With the mz Step you can select the distance between two chromatograms. Peaks within one half of the distance in positive direction and one half 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

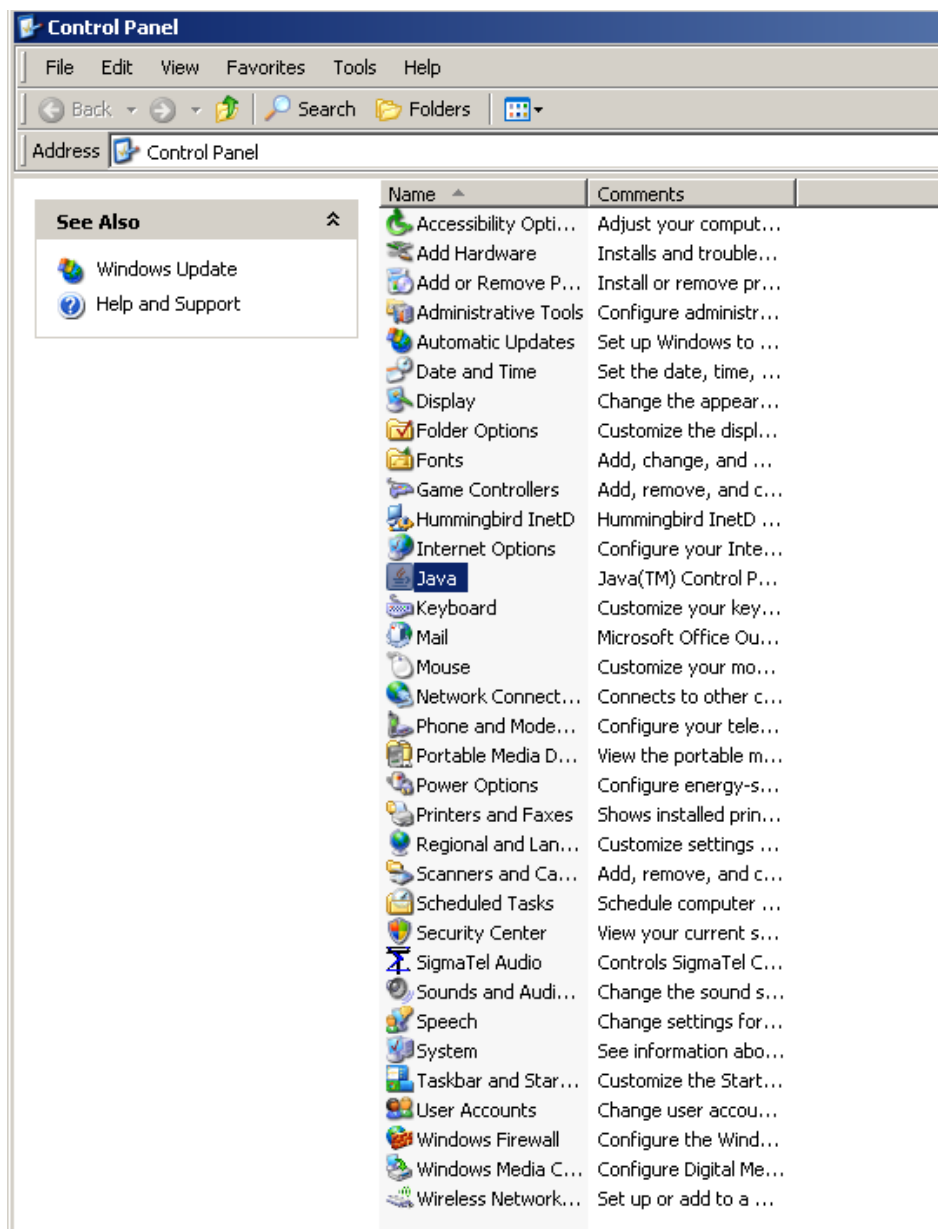
(Col)” the new peak finding algorithm is taken which quantifies peaks with saddle-points and foothills. The black “A=...” shows the stored area in the database the blue “A=...” shows the actually selected area for that peak. If a peak with the same boundaries is stored in the database the peak appears 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

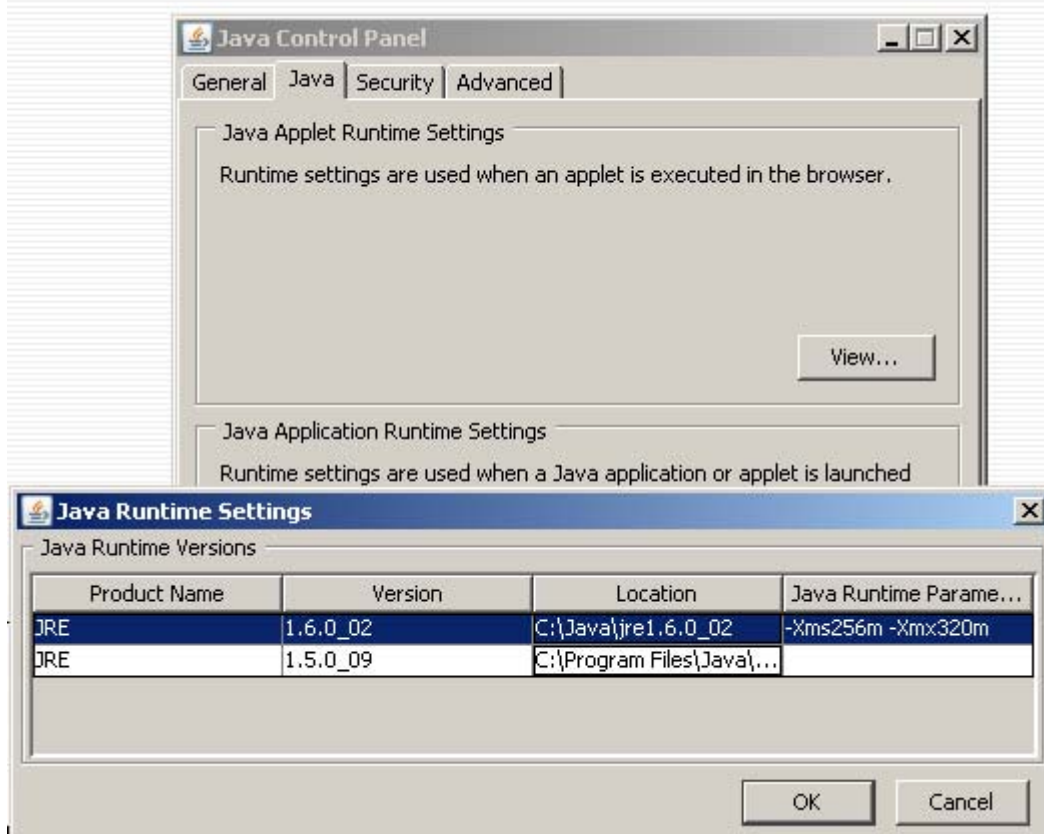
To run the 3D-viewer Java3D must be installed. You can download this from:

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

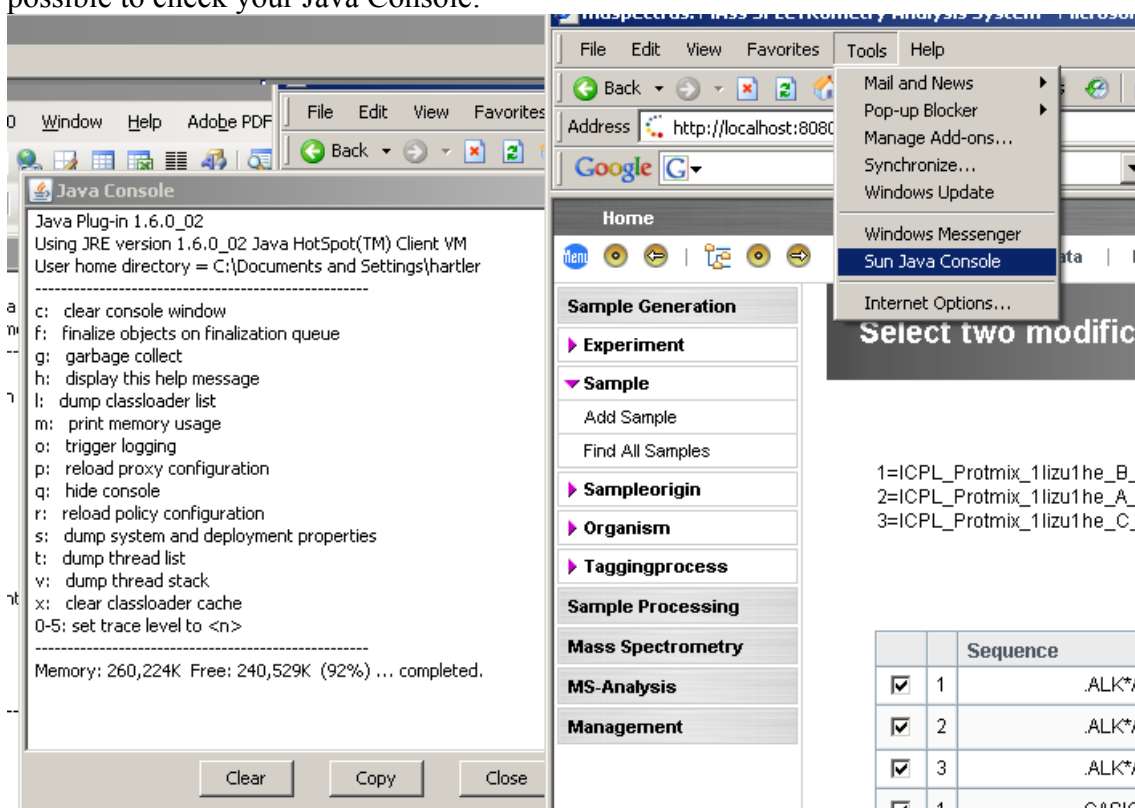
When you installed Java3D you have to reserve more memory for the applet. In Windows you have to go to “Control Panel” and then double-click on Java.



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:

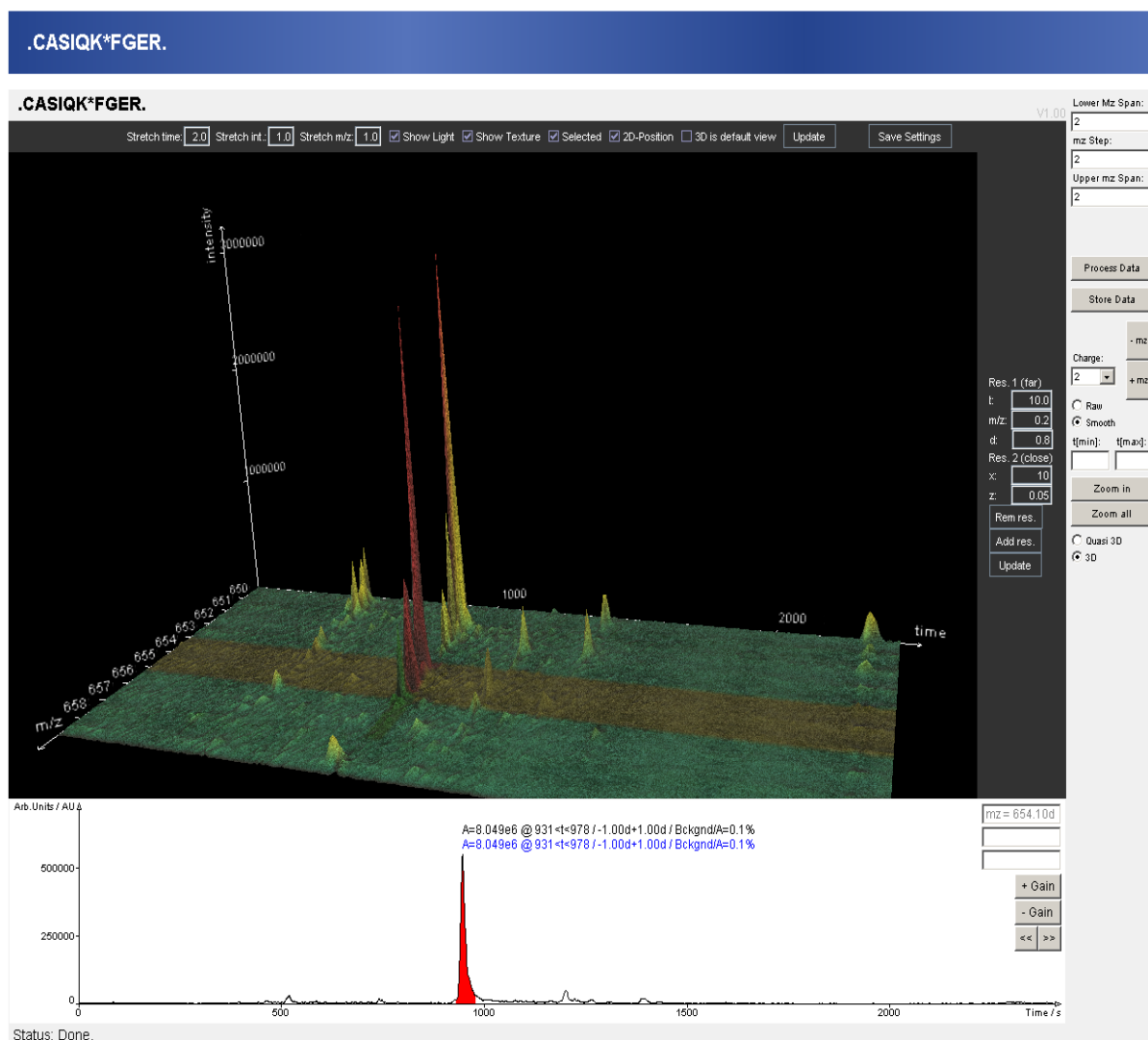


1=ICPL_Protmix_1lizu1he_B_
2=ICPL_Protmix_1lizu1he_A_
3=ICPL_Protmix_1lizu1he_C_

	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:

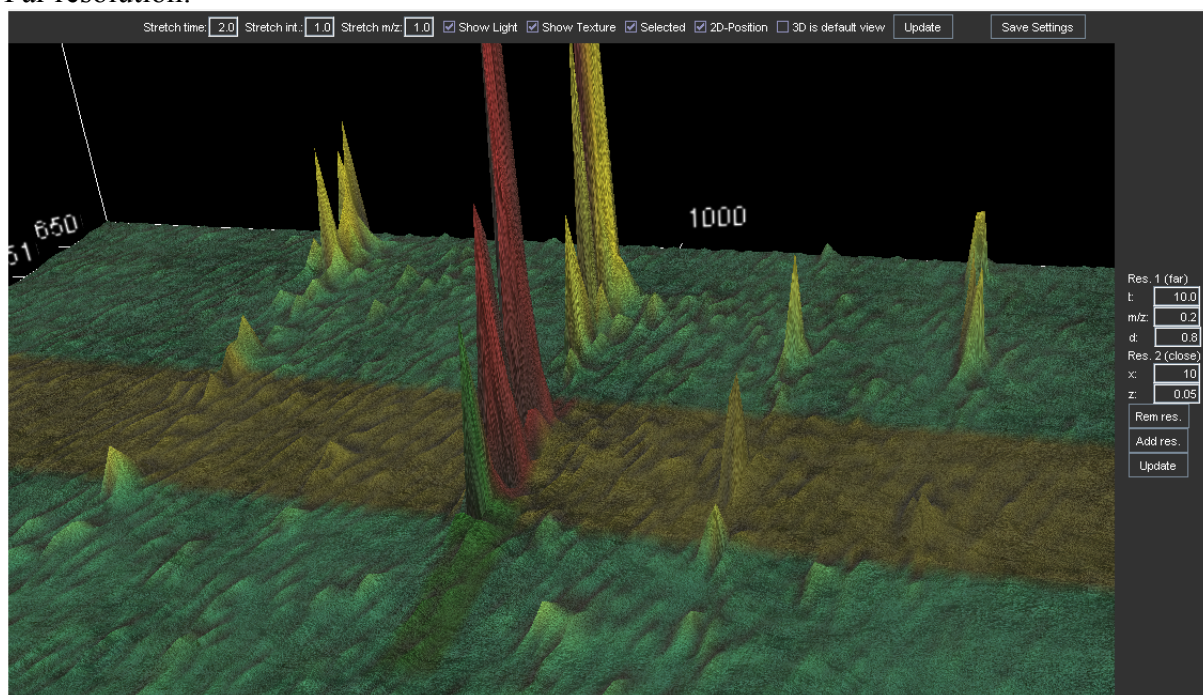


The memory used for this applet is mainly dependant on the resolution used and on effects like “Show Light” or “Show Texture”.

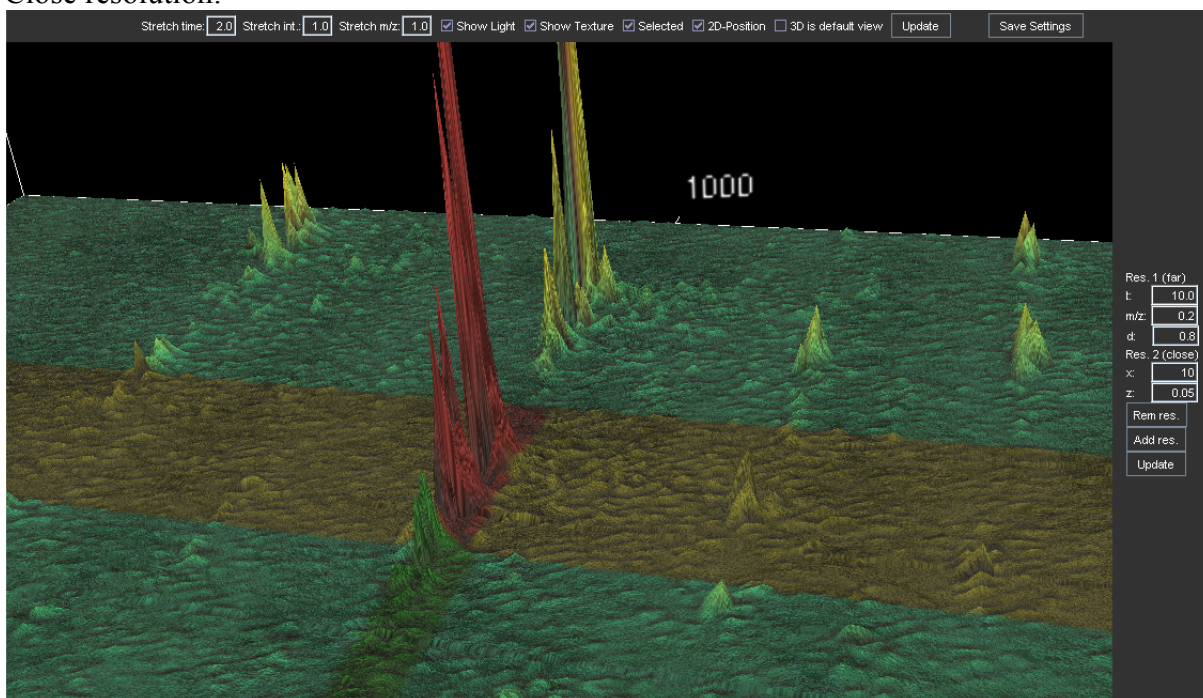
With the “Update” buttons you execute your changed settings.

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

