

The logo for QuPE consists of several overlapping, 3D-style blue trapezoidal shapes. The text 'QuPE' is rendered in a white, bold, sans-serif font with a slight drop shadow, positioned across the center of these shapes. The URL 'http://qupe.cebitec.uni-bielefeld.de' is written in a smaller, white, sans-serif font in the upper right area of the blue shapes.

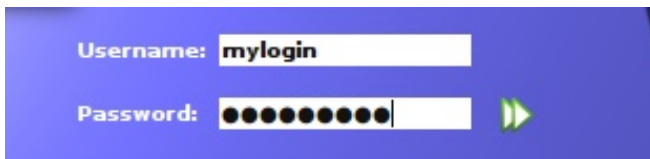
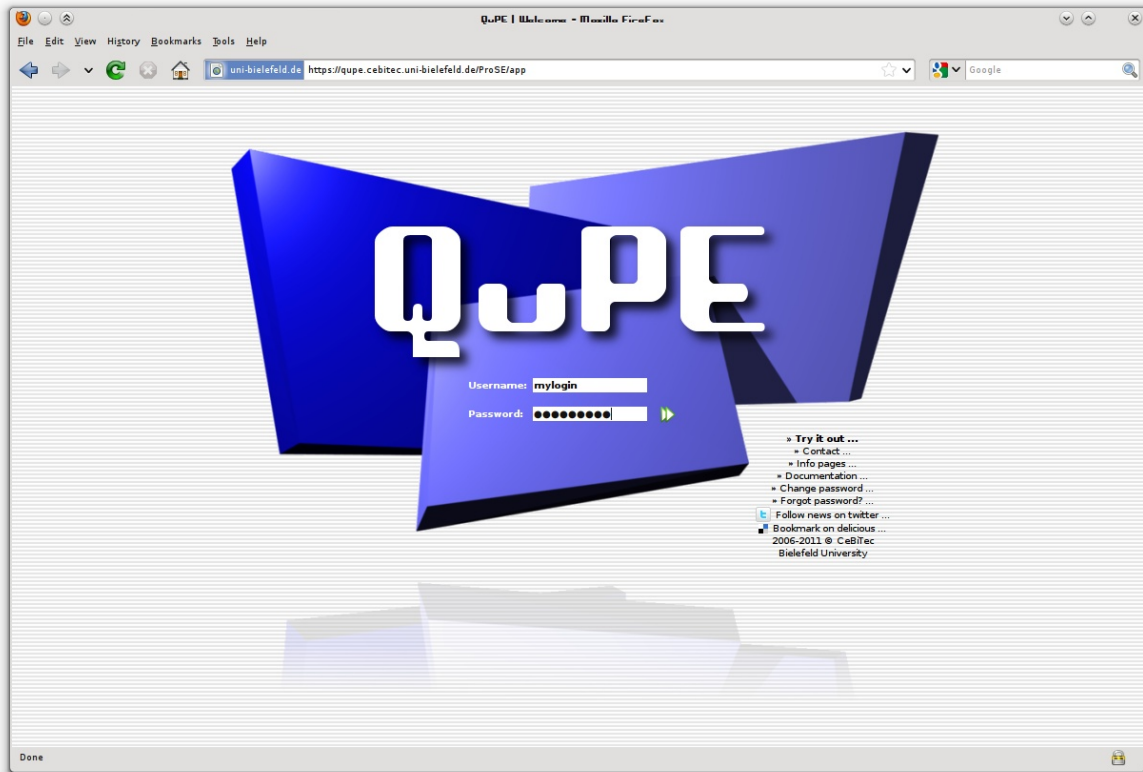
<http://qupe.cebitec.uni-bielefeld.de>

**QuPE**

A faint, light gray reflection of the QuPE logo is positioned below the main logo, mirroring its 3D trapezoidal structure.

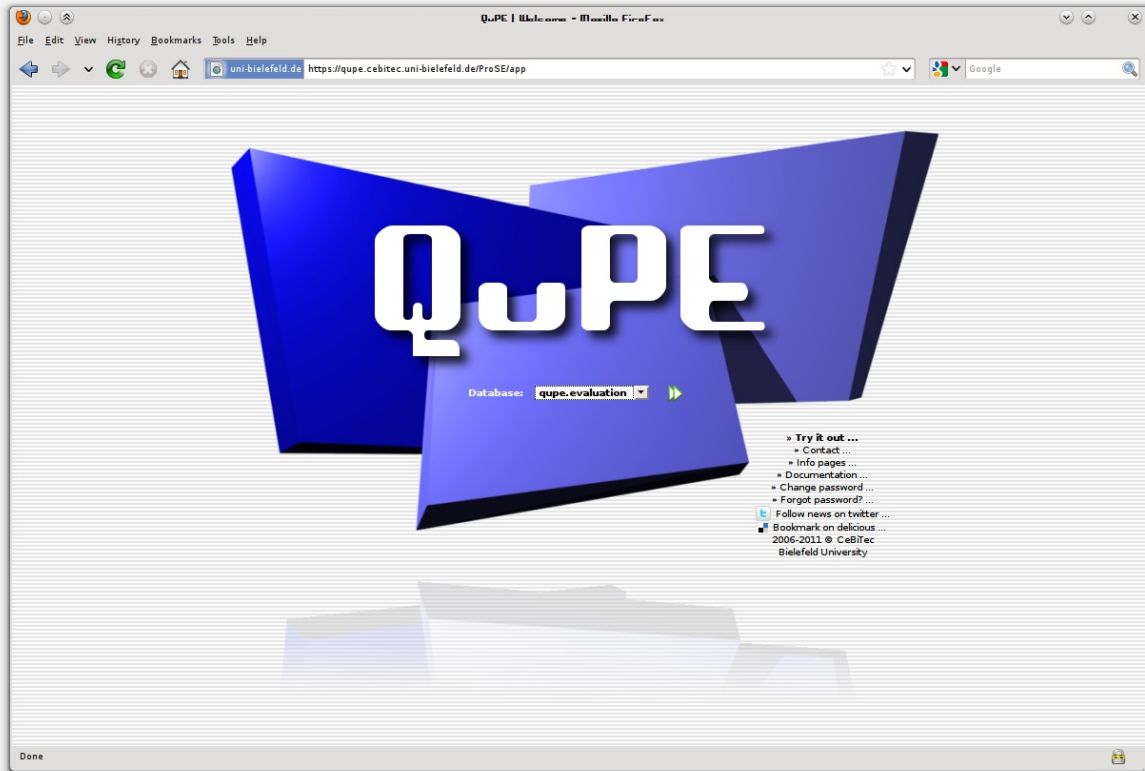
# A walk through QuPE

A guide through the computational analysis of isotope-labeled mass spectrometry-based quantitative proteomics data



In the following, we would like to introduce you to some of the functionality of QuPE - a rich internet application to store and analyze quantitative proteomics experiments. This walkthrough aims to guide through the system and demonstrates how to browse analysis results. QuPE is best displayed using Mozilla Firefox, but other browsers such as Google Chrome or Internet Explorer can, of course, also be used.

To **log into** the system, please first enter your **username** and **password** or click on the "**Try it out...**" link on the right side of the logo.

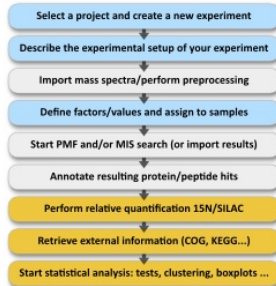


After log-in please choose a database. Please select for example "qupe.evaluation", to view the analysis results presented in "A guide through the computational analysis of isotope-labeled mass spectrometry-based quantitative proteomics data: an application study".

## Welcome to QuPE

### An Integrated Bioinformatics Environment for the Storage, Analysis and Integration of Proteomics Data

QuPE will accompany you in the performance of your mass spectrometry-based quantitative proteomics experiments. The rich internet application provides comprehensive data management and analysis functions including protein or peptide identification by database search, the calculation of protein abundance ratios, and, in particular, the statistical evaluation of quantification results.



Your work with QuPE usually begins with the creation of a new experiment. In QuPE, several experiments belong to a project, which in turn logically groups related experiments such as those of an individual working team. Differentiated access rights can be assigned to other users allowing them to read, modify or even delete your experiments as well as projects.

At second, you may want to describe your experimental setups to allow for future look-up and retrieval of information about the experiment. This is followed by the import of mass spectrometry data. Currently, the open source formats mzXML and mzData are supported as well as a proprietary format by Bruker for single-stage mass spectrometry (mainly used in-house).

PMF or MS search can be carried out by the integrated Mascot (TM) search engine. Alternatively, e.g. Sequest results may be imported. Search results can then be evaluated, either manually or automatically, to choose those proteins or peptides, respectively, that will be included in further analysis.

An important step is the description of your treatment: For an experiment one or more types of treatment, such as temperature or concentration of a substance, may be defined and assigned to the imported samples. If for example samples were taken in distinct time intervals, therefrom calculated abundance ratios will be grouped in separate datasets, that can then be compared to each other using statistical inference methods.

Furthermore, information from external resources can be integrated, for example to calculate the distribution of COG categories or to map identified proteins on KEGG pathways.

[Continue working on a project...](#)

[Create a new project...](#)

... what do you want to do?

[View documentation...](#)

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Information from external resources can be integrated, for example KEGG pathways.

[Continue working on a project...](#)



under the GNU General Public License (GPL).

Welcome to QuPE! The software helps to organize and manage your quantitative proteomics experiments: In QuPE, several experiments belong to a project, which in turn logically groups related experiments such as those of an individual working team. Differentiated access rights can be assigned to other users allowing them to read, modify or even delete your experiments as well as projects.

To proceed through the guide, please select "Continue working on a project...".

## Project Selection



A project in QuPE is a collection of all your data relevant to a specific topic. It usually consists of a number of individual experiments. Please chose whether you would like to continue your work on an already existing project - in that case please select a project from the list below - or begin a new project - then please select the appropriate action below or open the "Project" menu above and click on "Create a new project...".

Please select a project from the following list to continue your work on that project:

	Project Name	Created by	Description	#Experiments
	Evaluation project	Stefan Albaum	Project for the evaluation of statistical analysis methods for isotope-labeled mass spectrometry-based quantitative proteomics data.	3

Choose the following action to create a new project:



Create a new project...

## Project Selection



Please select a project from the follo

	Project Name
	Evaluation project

The following page lists all projects within the selected database - given, of course, that you have the appropriate access rights. Usually, you will only want to create a new personal or workgroup-related project in the beginning of your work with QuPE. Afterwards, you probably only want to create new experiments within this project.

To continue your work on an existing project, just click on the projects entry in the list, in our case the yellow-highlighted "Evaluation project".

## Project Overview / Experiment Selection



Here you can see an overview of your project which usually consists of one or more experiments. You can either continue your work on an already existing experiment by selecting it from the list below, or create a new one by clicking on the appropriate button or choosing "Create a new experiment..." from the "Experiment" menu above. In addition, you can modify various parameters of your project such as access rights or your project's name and description.



### Information about current project "Evaluation project":

**Owner:** Stefan Albaum (7 users have access privileges to this project)  
**Description:** Project for the evaluation of statistical analysis methods for isotope-labeled mass spectrometry-based quantitative proteomics data.

Please select an experiment from the following list to continue your work on that experiment:

	Experiment Name	Created by	Description	Organism(s)	Experimental setup	Samples imported	Proteins annotated	Performed analyses
	Salt stress adaption	Stefan Albaum	MS-data of H. Hahne et al. (2010), Journal of Bacteriology: B. subtilis, salt stress adaption, 15 datasets, 3 time points taken during cell growth, 3 biological replicates, each 12 LC-MS/MS runs	Bacillus subtilis [GenDB_B_amyloliquefaciens-2.2]	-	180	1445	33
	Systems-wide profiling	Stefan Albaum	MS-data of A. Otto et al. (2010), Nature communications: Systems-wide temporal proteomic profiling in glucose-starved Bacillus subtilis, 5 time points taken during cell growth, 3 biological replicates, cytosolic fraction	Bacillus subtilis [GenDB_B_amyloliquefaciens-2.2]	-	292	2472	19
	Adaptation to benzoate	Stefan Albaum	MS-data of U. Haussmann et al. (2009), Proteomics: Physiological adaptation of Corynebacterium glutamicum to benzoate as alternative carbon source - a membrane proteome-centric view, benzoat as sole carbon and energy source, only first biological replicate	Corynebacterium glutamicum [GenDB_C_glut_ZFG-2.2]	-	22	712	15

Choose the following action to create a new experiment:

Create a new experiment...

View and/or modify properties of the current project "Evaluation project":

View jobs of the current project...
 Change permissions of the current project...
 Edit the current project...
 Delete the current project...
 Change project...

Please select an experiment from the follow

	Experiment Name	Created by	Desc
	Salt stress adaption	Stefan Albaum	MS-da subtilis cell gr
	Systems-wide profiling	Stefan Albaum	MS-da System Bacillu replica
	Adaptation to benzoate	Stefan Albaum	MS-da adapt. altern. benzo replica

After selection of a project, again a list - here of all experiments belonging to the selected project - is displayed. In this case, three experiments are shown which correspond to the three experiments of the referred manuscript: experiment A is named "Salt stress adaption", experiment B "Systems-wide profiling", and experiment C "Adaption to benzoate". Choose one of the experiments, e.g. the first, to browse its results.

## Experiment Overview

In QuPE, an experiment generally corresponds to a number of samples you would like to analyse or, better to say, runs you performed on a mass spectrometry instrument. If you for example analysed your data using a MALDI-TOF mass spectrometry instrument, you might want to combine several related matrices in one experiment.

By selecting an experiment from the list below and choosing an action you can...

- Describe the experimental setups to allow for future look-up and retrieval of information about the experiment

- Import, browse and compare mass spectrometry data, perform PMF or MIS search by the integrated Mascot (TM) search engine, or import e.g.

Sequence results

- Evaluate database search results, either manually or automatically, and choose those proteins or peptides that will be included in further analysis

- Describe the treatment of the samples such as different temperatures or concentration of a substance, and group the imported samples accordingly

- Perform analysis or integrate data from external resources, e.g. to calculate the distribution of COG categories or to map identified proteins on KEGG pathways



### Information about current experiment "Salt stress adaption":

**Owner:** Stefan Albaum (7 users have access privileges to this experiment)  
**Description:** MS-data of H. Hahne et al. (2010). Journal of Bacteriology: B. subtilis, salt stress adaption, 15 datasets, 5 time points taken during cell growth, 3 biological replicates, each 12 LC-MS/MS runs  
**Organism(s):** Bacillus subtilis [GenDB\_B\_amyloliquefaciens-2.2]

<b>Number of imported samples/runs:</b>	180
<b>Experimental setup description:</b>	-
<b>Currently assigned type(s) of treatment:</b>	Time
<b>Number of hits found in PMF/MIS searches (or imported):</b>	181959
<b>Number of annotated proteins:</b>	1445
<b>Number of performed analyses:</b>	33

Please choose one of the following actions:



**Import data, browse mass spectra, perform database search (PMF/MIS)...**



**Describe experimental setup (LIMS)...**



**Describe treatment and group samples...**



**Evaluate database search results (FDR calculation, annotation)...**



**Perform analysis and view results - quantification, statistics, data integration...**

View and/or modify properties of the current experiment "Salt stress adaption":



**View jobs of the current experiment...**



**Change permissions of the current experiment...**



**Edit the current experiment...**



**Delete the current experiment...**



**Change experiment...**

<b>Number of imported samples/runs:</b>	180
<b>Experimental setup description:</b>	-
<b>Currently assigned type(s) of treatment:</b>	Time
<b>Number of hits found in PMF/MIS searches (or imported):</b>	181959
<b>Number of annotated proteins:</b>	1445
<b>Number of performed analyses:</b>	33

An experiment generally corresponds to a number of samples you would like to analyse or, better to say, runs you performed on a mass spectrometry instrument. If you for example analysed your data using a MALDI-TOF mass spectrometry instrument, you might want to combine several related matrices in one experiment, or, in case of LC-MS/MS, several runs.

The blue information box on the left side displays information about the current number of imported samples, observed database hits, and performed analysis.



## Basic navigation in QuPE

In general, all navigation in QuPE can be done using the menu in the title bar:

- Use the Application menu to change the database and to log out
- The project as well as the experiment menu allow to change your current project or experiment, respectively, but also the creation of a new one
- Other menus provide options for data import, export, and allow to start analyses
- Have a look at the help menu to browse related resources and more documentation (please allow **pop-up windows** therefore)

The status bar allows to quickly navigate to the project or experiment overview page by clicking on the appropriate entry. If a specific spectrum (02\_cvvb.mzxml/2879 in our example) or protein (e. g. Cg2705) has been selected somewhere, a click will directly provide additional information.



Two very important actions:

Select the "Return to experiments overview page..." to get back to the overview and browse to another page, and "Change experiment..." to switch to another experiment.



Application Project Experiment Tools Settings Help Fri, 29 Apr 2011

qupe user 1 qupe.evaluation Evaluation project Salt stress adaption

## Experiment Overview

In QuPE, an experiment generally corresponds to a number of samples you would like to analyse or, better to say, runs you performed on a mass spectrometry instrument. If you for example analysed your data using a MALDI-TOF mass spectrometry instrument, you might want to combine several related matrices in one experiment. By selecting an experiment from the list below and choosing an action you can...

Describe the experimental setups to allow for future look-up and retrieval of information about the experiment

Import, browse and compare mass spectrometry data, perform PMF or MIS search by the integrated Mascot (TM) search engine, or import e.g. Sequest results

Evaluate database search results, either manually or automatically, and choose those proteins or peptides that will be included in further analysis

Describe the treatment of the samples such as different temperatures or concentration of a substance, and group the imported samples accordingly

Perform analysis or integrate data from external resources, e.g. to calculate the distribution of COG categories or to map identified proteins on KEGG pathways

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**Information about current experiment "Salt stress adaption":**

Owner: Stefan Albaum (7 users have access privileges to this experiment)

Descriptions: MS-data of H. Hahne et al. (2010). Journal of Bacteriology. B. subtilis, salt stress adaption, 15 datasets, 5 time points taken during cell growth, 3 biological replicates, each 12 LC-MS/MS runs

Organism(s): Bacillus subtilis [GenDB\_B\_amyloliquefaciens-2.2]

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**Number of imported samples/runs:** 180

**Experimental setup description:** -

**Currently assigned type(s) of treatment:** Time






**Number of hits found in PMF/MIS searches (or imported):** 181959

**Number of annotated proteins:** 1445

**Number of performed analyses:** 33






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**Please chose one of the following actions:**

-  **Import data, brows**
-  **Describe experimer**
-  **Describe treatment**
-  **Evaluate database**
-  **Perform analysis ar**


---


**Please chose one of the following actions:**


-  **Import data, browse mass spectra, perform database search (PMF/MIS)...**
-  **Describe experimental setup (LIMS)...**
-  **Describe treatment and group samples...**
-  **Evaluate database search results (FDR calculation, annotation)...**
-  **Perform analysis and view results - quantification, statistics, data integration...**

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View and/or modify properties of the current experiment "Salt stress adapti

 View jobs of the current experiment...

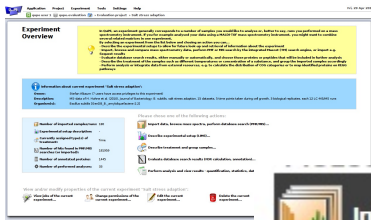
 Change permissions of the current experiment...

 Edit the current experiment...

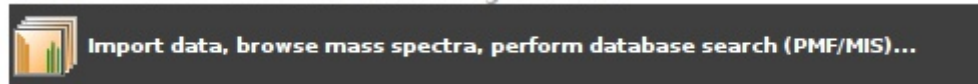
Basically, the workflow of an experiment in QuPE consists of five steps:

1. Import of mass spectrometry data followed by a PMF or MIS search using the integrated Mascot (TM) search engine or import e.g. of Sequest results
2. Description of the experimental setups to allow for future look-up and retrieval of information about the experiment
3. Definition of factors and values to organize samples for further analysis steps. An example for a factor would be "time" with levels 1, 2, and 3h
4. Evaluation of search results, either manually or automatically to choose a set of proteins or peptides, respectively, that will be included in further analysis
5. Calculation of abundance ratios, statistical analysis, integration of annotation data from external resources, e.g. to calculate the distribution of COG categories or to map identified proteins on KEGG pathways

**Please note:** the following three pages explain how to browse mass spectra, to group samples, and to evaluate database search results (PMF/MIS). You may want to skip over these pages and directly proceed with the walk through the analysis results.



On the experiment overview page, select the action "Import data, browse mass spectra, perform database search..." to browse imported mass spectra...



Application Project Experiment Import Search Export Tools Settings Help Fri, 29 Apr 2011

qupe user 1 qupe-evaluation Evaluation project Salt stress adaption 080514\_o3\_u2\_hh\_salk-r2-m010\_01.mzxml/7377

Please select a sample to display corresponding mass spectra in the right frame...

Search spectrum by id:

Sample	Size
080514_o3_u2_hh_salk-r2-m010_01.mzxml	4712
080514_o3_u2_hh_salk-r2-m010_02.mzxml	4468
080514_o3_u2_hh_salk-r2-m010_03.mzxml	4668
080514_o3_u2_hh_salk-r2-m010_04.mzxml	4701
080514_o3_u2_hh_salk-r2-m010_05.mzxml	4717
080514_o3_u2_hh_salk-r2-m010_06.mzxml	5261
080514_o3_u2_hh_salk-r2-m010_07.mzxml	4840
080514_o3_u2_hh_salk-r2-m010_08.mzxml	4811
080514_o3_u2_hh_salk-r2-m010_09.mzxml	4770
080514_o3_u2_hh_salk-r2-m010_10.mzxml	4769
080514_o3_u2_hh_salk-r2-m010_11.mzxml	4553
080514_o3_u2_hh_salk-r2-m010_12.mzxml	4459

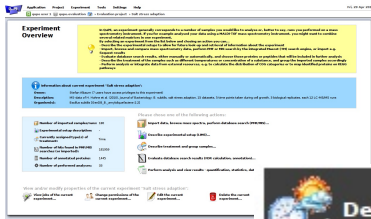
< Previous 1 of 15 Next >

MS/MS spectra of currently selected parent spectrum (ID: 7375):

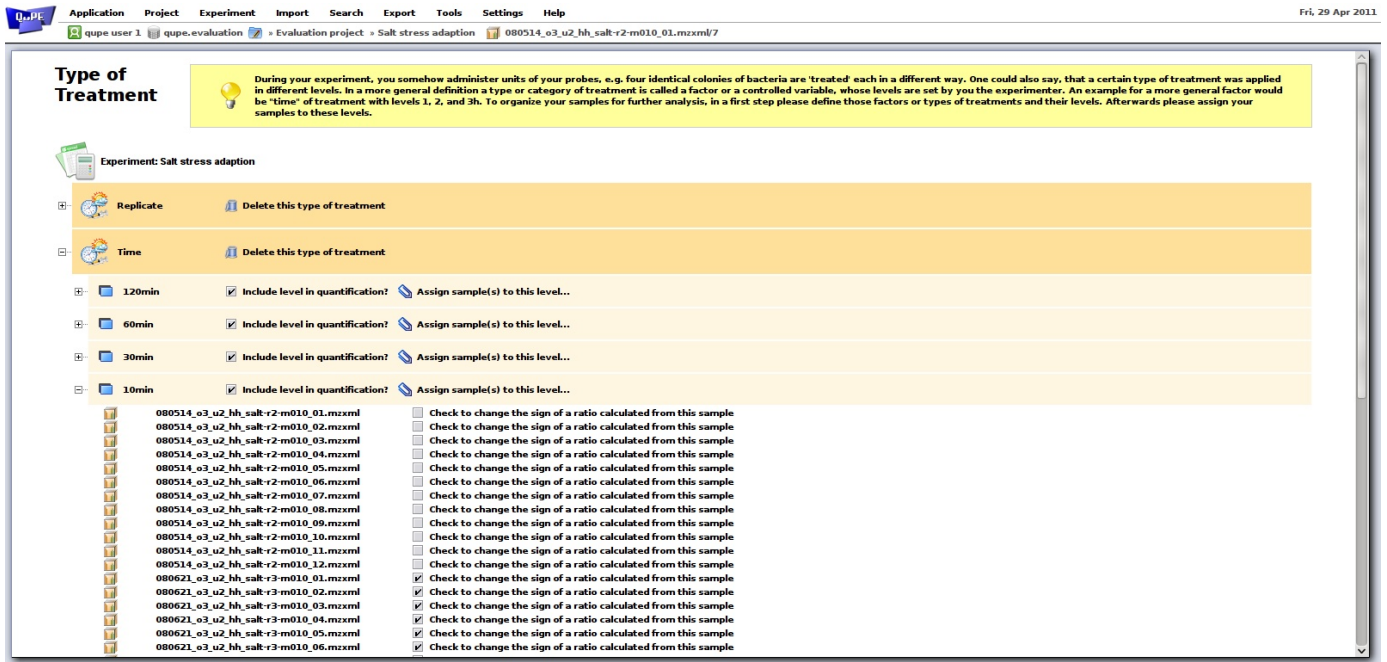
ID	Status	MS <sup>n</sup>	Time	Type	Precursor m/z	Precursor intensity	Precursor charge	Hit(s) / Peptide(s)
7376	preprocessed	2	5333.41 seconds	discrete	421.75793	780431.0	2	
7377	preprocessed	2	5333.88 seconds	discrete	635.2766	306850.0	3	[P02968] Flagelin - Bacillus subtilis (scores: 29, -)
7378	preprocessed	2	5334.59 seconds	discrete	541.94745	233939.0	2	[P02968] Flagelin - Bacillus subtilis (scores: 119, -)

show/hide spectrum "7377"

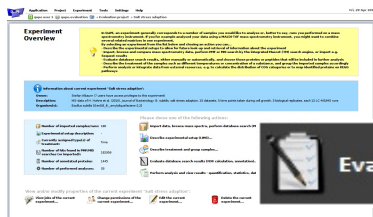
Working with mass spectra: In the left sidebar all imported samples (e. g. LC runs) are displayed, select one to browse the corresponding mass spectra. In general, for each imported file (mzData, mzXML,..) a separate sample has been created. On the right side all spectra belonging to the selected sample will be displayed. This includes MS level one spectra, and - if applicable - the child spectra (MS2, SIM, Zoom, etc.) associated to the selected MS1 scan. Buttons below the depicted peak lists provide zoom functionality. Checkboxes beside the spectrum allow to partly hide peak lists, for example to select only the precursor positions.



Any analysis demands grouping of samples which have been measured under the same conditions. Therefore, please choose the action "Describe treatment and group samples..." on the experiments overview page.



Before any analysis such as a statistical test can be performed, QuPE needs to know which samples have been measured under the same conditions. This is, for example, a distinct time point, a strain - e. g. mutant or wildtype -, or a specific growth medium. On this page, the model or basis of the experiment is described and set up. This will then be used in any further analysis, i. e. if abundance ratios are calculated these will be grouped into datasets according to the here described model, an analysis of variance will refer to this model, as well as a cluster analysis that will group the input data accordingly.



QuPE allows the import of search results, e. g. in form of a DTASelect-filter file, and has an integrated Mascot search engine to perform Peptide Mass Fingerprinting and MS/MS ion search.

Evaluate database search results (FDR calculation, annotation)...

Click on "Evaluate database search results..." to browse and work on all observed database hits.

**Search Results**

Here you are presented a list of all search results either found by Mascot(C) or imported e.g. from Sequest(C). On this page, you may sort, filter, and review the peptide or protein hits. It is the concept of QuPE, that a hit, before it is included in further analysis, has to be annotated with a level of certainty. This may either be done manually by selecting one or more hits from the list below and pressing the "Annotate..." button, or automatically utilizing the appropriate function from the "Search" menu above.

Please note, that dependent on the source of the data, either Mascot or Sequest scores are available. To perform further analysis based on the annotated proteins please switch to "Work on proteins..." utilizing the "Experiment" menu. If you want to have a look at the mass spectrum belonging to a potentially identified protein or peptide, simply select a hit from the list below and select "Work on ms spectra...", again utilizing the "Experiment" menu.

**Protein:** P02968 Sample/Spectrum: 080514\_o3\_u2\_hh\_salt-r2-m010\_01.mzxml / 7373

Flagellin - Bacillus subtilis  
 MKRHMEALALRILRISGMSASQSRDELSSGLRMRAGDAAAGLAIENCRHGRGLRGLRNSKMSNGSLSLDTAGAL  
 TETNALLQVRELVYVAGGTGTQDKATDLQSLQDELSALYDEIQGISMRTEHGKQLRGLTYKQDTATPAHOKNLYFQIG  
 ANATQOISVYIEDNGADALGIKEADGSLAALHSYVDLDTFRADNLAFTDIFGTRALKVYDEALINQVSSORAKLGAQVN  
 RLERTLNLKSAQGLRLLAASRISQDVRHMERSEFTQWELSSQVRLRANRQPNVLLKLR  
 Legend: selected peptide hits / other (annotated) peptide hits  
 Coverage: 96.4% (9369 peptides)  
 Coverage calculation method: annotated peptide hits / peptide hits found in the same search/import

**MS/MS ion search:** listed below: all hits found / for the same protein (P02968) / for the same spectrum / in the same search / in this experiment

Fdr	Sequence	Charge	Modifi-cations	Prot. Score	Mascot	Thres-hold	Coverage	X/Corr	deltCN	Sp	M+H+	expMr	calcMr	m. cl.	Sample/ Spectrum	Spectrum hits
0.0	K.FADNAADTADIG...	3.0		2594.0	25.0	22.0	30.0	-	-	-	628.2959	1881.9658	1881.8745	0	080514_o_010_01.mzxml/7373	1
0.0	K.FADNAADTADIG...	2.0		2594.0	119.0	22.0	30.0	-	-	-	941.941	1881.8674	1881.8745	0	080514_o_010_01.mzxml/5130	1
0.0	K.FADNAADTADIG...	2.0		2594.0	119.0	22.0	30.0	-	-	-	941.9412	1881.8678	1881.8745	0	080514_o_010_01.mzxml/5130	1
0.0	K.FADNAADTADIG...	2.0		2594.0	133.0	22.0	30.0	-	-	-	941.942	1881.8694	1881.8745	0	080514_o_010_01.mzxml/5409	1
0.0	K.FADNAADTADIG...	2.0		2594.0	131.0	22.0	30.0	-	-	-	941.9429	1881.8712	1881.8745	0	080514_o_010_01.mzxml/5164	1
0.0	K.FADNAADTADIG...	2.0		2594.0	122.0	22.0	30.0	-	-	-	941.9435	1881.8726	1881.8745	0	080514_o_010_01.mzxml/4854	1
0.0	K.FADNAADTADIG...	2.0		2594.0	124.0	22.0	30.0	-	-	-	941.9445	1881.8744	1881.8745	0	080514_o_010_01.mzxml/6745	1
0.0	K.FADNAADTADIG...	2.0		2594.0	117.0	22.0	30.0	-	-	-	941.9445	1881.8744	1881.8745	0	080514_o_010_01.mzxml/5666	1
0.0	K.FADNAADTADIG...	2.0		2594.0	120.0	22.0	30.0	-	-	-	941.9448	1881.875	1881.8745	0	080514_o_010_01.mzxml/4586	1

The list on the left side displays all proteins found in database searches. Click on a table header to sort the list, e.g. by the number of observed hits. Select a protein from the list to show all related database hits (protein hits in case of PMF, peptide hits in case of MIS) on the right side of the page. Again you may click on the table headers to sort the list. Above the list of all protein/peptide hits options are provided for filtering. Instead of having a look at all hits found for the currently selected protein you may thereby investigate whether other hits have been found for the same spectrum. Additional information is displayed when a hit was selected: If appropriate accession numbers are found, links to uniprot or ncbi will be available, and in case search results were obtained by a Mascot search, links to these search results will be shown.

Please click on "Perform analysis and view results..." on the experiments overview page to start quantification of your proteins, conduct a statistical test or a hierarchical clustering.

**Proteins / Analysis Results**

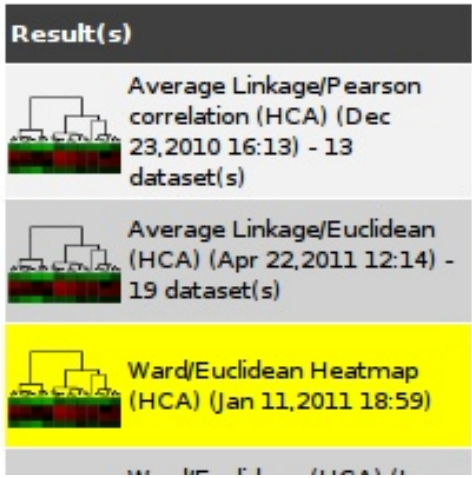
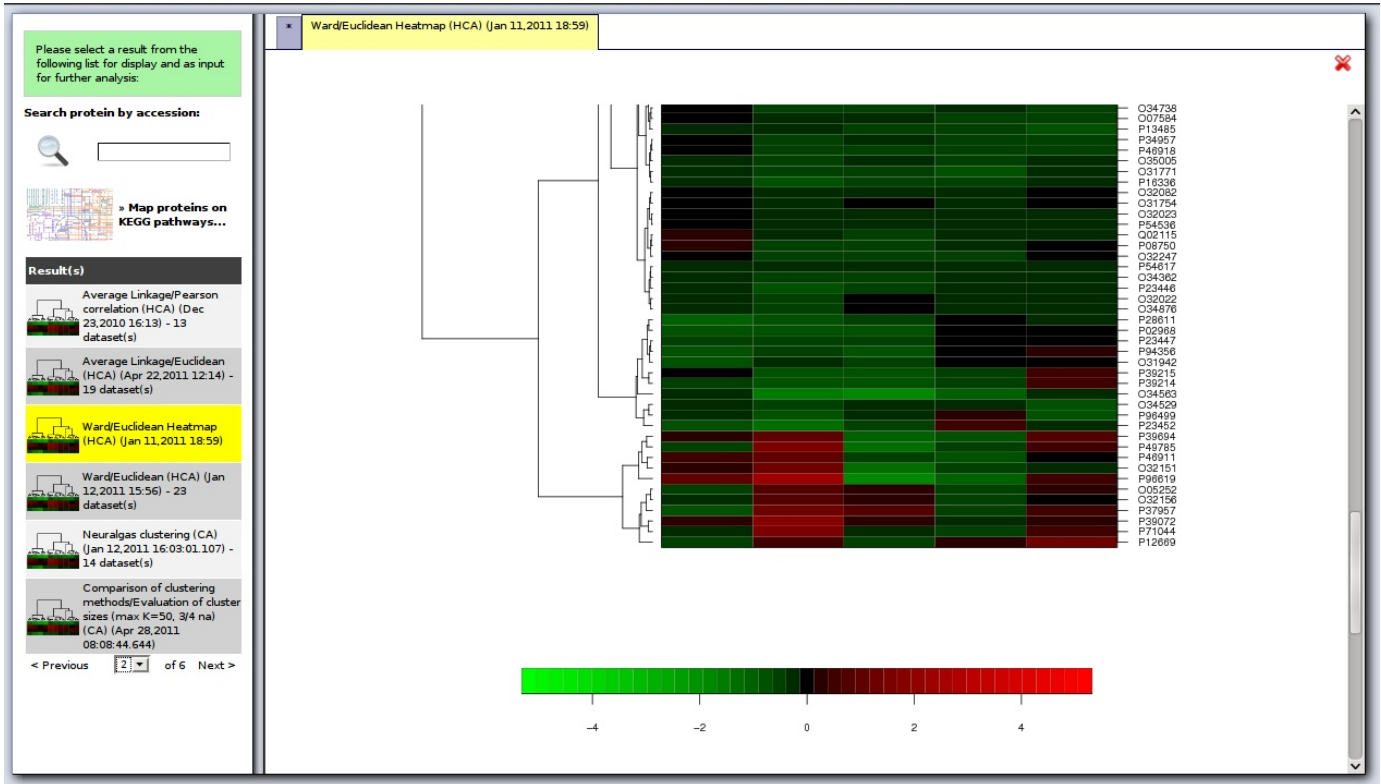
Performing a PMF or MS/MS search on your mass spectra results in a number of significant database hits. As soon as one or more observed protein or peptide hits, respectively, have been identified - in terms of QuPE they are annotated, either manually or by the auto annotator - these "approved" protein(s) are included in the following protein list of your experiment. If you import DTASelect-filter lists, those proteins are automatically added. Based on these proteins further analysis can be performed. Therefore, please select a function from the "Analysis" menu above. The results of such an analysis are afterwards displayed in the list on the left hand side of this page. Select an item from the list, and all results such as datasets or illustrations are opened in a new tab page. Please note: Whenever an analysis (or export) function depends on the results of another analysis, e.g. the variance analysis depends on the a previously performed quantification, please first select this result in the list, which is then marked yellow, and afterwards start the second, dependent analysis function.

Accession	Alternative names	MW	pI	#HRs	#Unique peptides	Description	Comment	COG/KOG	EC
005227	MRPG_BACSU, mrpG, yuFB, BSU31660, NP_391044.1	19617.0	9.03	35	4	Nal+(H)(+) antiporter subunit G - Bacillus subtilis Nal+(H)(+) antiporter subunit G;Multiple resistance and pH homeostasis protein G;Mrp complex subunit G Nal+(H)(+) antiporter subunit G;Mrp complex subunit G;Multiple resistance and pH homeostasis protein G		P	
005228	MRPF_BACSU, mrpF, yuFC, BSU31650, NP_391043.1	10224.0	8.15	3	1	Nal+(H)(+) antiporter subunit F - Bacillus subtilis Nal+(H)(+) antiporter subunit F;Multiple resistance and pH homeostasis protein F;Mrp complex subunit F;Sodium-cholate efflux protein mrpF Nal+(H)(+) antiporter subunit F;Mrp complex subunit F;Multiple resistance and pH homeostasis protein F;Sodium-cholate efflux protein mrpF		P	
005229	MRPD_BACSU, mrpD, yuFD, BSU31630, NP_391041.2	53342.0	9.23	2	1	Nal+(H)(+) antiporter subunit D - Bacillus subtilis Nal+(H)(+) antiporter subunit D;Multiple resistance and pH homeostasis protein D;Mrp complex subunit D Nal+(H)(+) antiporter subunit D;Mrp complex subunit D;Multiple resistance and pH homeostasis protein D		CP	1.6.5.3
005239	YUGJ_BACSU, yugJ, BSU31370, NP_391015.1	42706.0	5.35	4	2	Probable NADH-dependent butanol dehydrogenase 1 - Bacillus subtilis Probable NADH-dependent butanol dehydrogenase 1		C	
005248	YUGP_BACSU, yugP, BSU31310, NP_391009.1	24679.0	8.89	85	4	Putative uncharacterized protein yugP - Bacillus subtilis Putative membrane protease yugP		R	
005249	YUFK_BACSU, yuFK, BSU31510, NP_391029.1	23219.0	9.1	6	1	Uncharacterized protein yuFK - Bacillus subtilis Uncharacterized membrane protein yuFK			
005250	MALK_BACSU, malK, yuFL, BSU31520, NP_391030.1	58899.0	6.86	20	9	Sensor protein malK - Bacillus subtilis Sensor histidine kinase malK;Malate kinase sensor		T	2.7.13.3
005252	YUFIN_BACSU, yuFN, BSU31540, NP_391032.1	37326.0	5.03	835	35	Uncharacterized Ipprotein yuFN precursor - Bacillus subtilis Uncharacterized Ipprotein yuFN		R	
005253	YUFO_BACSU, yuFO, BSU31550, NP_391033.1	56265.0	7.25	255	30	Putative uncharacterized protein yuFO - Bacillus subtilis Uncharacterized ABC transporter ATP-binding protein yuFO		R	
005254	YUFP_BACSU, yuFP, BSU31560, NP_391034.1	36820.0	9.18	9	1	Putative uncharacterized protein yuFP - Bacillus subtilis Uncharacterized ABC transporter permease protein yuFP		R	

< Previous | 10 | Page | 1 | of 145 Next >

[Add/Edit comment of the selected protein...](#)
[Retrieve GenDB annotation...](#)
[Show measurements for the selected protein...](#)

After mass spectra have been imported in QuPE, a database search has been conducted (or protein identifications have been imported), resulting hits have been processed (e. g. filtered using an FDR threshold), and the model of the experiment has been described (i. e. samples recorded under the same condition have been grouped together), next steps are quantification, data integration and analysis. Found on this page is, firstly, a table showing all identified ('annotated') proteins. Any further analysis will be based on this list of proteins. Secondly, different kinds of analysis can be started and the results e. g. of a protein quantification, a statistical test or a hierarchical clustering can be viewed. In our example, the results for experiment A "Salt stress adaption" are shown. To begin with, a tool has been invoked to enrich our knowledge of the identified proteins with information from "other" databases like uniprot, ncbi and our gene annotation system GenDB.



If a result has been selected the main window on the right side utilizes tabs to display the selected results object and other information. In our example, the heatmap resulting from a hierarchical cluster analysis using Ward and Euclidean distances is displayed. Click on the tab named "\*" to switch back to the protein overview. To browse all results of an experiment, use the table navigation and switch to the "previous" or the "next" page of results. In the beginning always the latest analysis results on the last page are displayed.

Application Project Experiment Search Import Export Analyse Tools Settings Help

qupe user 1 qupe.evaluation Evaluation project Salt stress adaption contamination\_K1C9\_HUMAN Quantification r>... (Oct 15,2010 16:49)

Ward/Euclidean Heatmap (HCA) (Jan 11,2011 18:59) Quantification r>0.6, exact 0.01 (Oct 15,2010 16:49) R:contamination\_K1C9\_HUMAN

Please select a result from the following list for display and as input for further analysis:

Search protein by accession:

Map proteins on KEGG pathways...

Result(s)

Quantification r>0.6, exact 0.01 (Oct 15,2010 16:49) - 5 dataset(s)

Average Linkage/Pearson correlation (HCA) (Dec 23,2010 16:36) - 92 dataset(s)

Average Linkage/Uncentered pearson (HCA) (Dec 23,2010 16:49) - 66 dataset(s)

Shapiro-Wilk test of normality (on residues) (Dec 17,2010 11:29) - 1 dataset(s)

Map of expression values on KEGG pathways (Dec 18,2010 14:30) - 1 dataset(s)

Average Linkage/Uncentered pearson (HCA) (Dec 23,2010 16:10) - 13 dataset(s)

< Previous 1 of 6 Next >

Protein/Peptide	Ratio(M)	Intensity(A)	Peptide(s)	Sample	Unlabeled Start	Labeled Stop	Labeled Start	Labeled Stop
contamination_K1C9_HUMAN	2.4062238	0.84655666	K.SDLEM*QYETLQEELM*ALK.K.3	r2-m060_09.mzxml	734.83997	736.70996	741.17384	743.70996
contamination_K1C9_HUMAN	3.461761	1.2257456	R.GGSGGSYGSGGSGGGYGGGSGSR.G.3	080517_o3_u2_hh_salt-r2-m120_01.mzxml	597.7133	599.25	605.38	607.9166
contamination_K1C9_HUMAN	4.050082	1.5978116	R.GGSGGSYGSGGSGGGYGGGSGSR.G.3	080517_o3_u2_hh_salt-r2-m060_09.mzxml	597.7133	599.25	605.38	607.9166
contamination_K1C9_HUMAN	5.327909	6.5319214	R.GGSGGSFYSGGSGGGFASLSLGGFGGSGSR.G.2(3)	080722_o1_hh_salt-r4-m060_06.mzxml	1352.905	1355.61	1368.905	1373.11

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Treatment (factors and values) assigned to the following dataset:

Time 120min

Protein/Peptide	Ratio(M)	Intensity(A)	Peptide(s)	Sample	Unlabeled Start	Labeled Stop	Labeled Start	Labeled Stop
contamination_K1C9_HUMAN	5.022376	2.2019625	K.DIENQYETQIQIEHEVSSSGQEVQSSAK.E.4	080517_o3_u2_hh_salt-r2-m120_01.mzxml	816.70496	818.4075	825.45496	827.9075
contamination_K1C9_HUMAN	2.9935234	2.138866	R.MTLDDFR.I.2	080517_o3_u2_hh_salt-r2-m120_01.mzxml	449.03	450.735	453.03	455.735
contamination_K1C9_HUMAN	-5.2503934	3.6554306	R.GGSGGSYGSGGSGGGYGGGSGSR.G.2	080625_o3_u2_hh_salt-r3-m120_05.mzxml	896.165	898.37	907.665	911.37
contamination_K1C9_HUMAN	0.43620828	1.5726392	K.STM*QELNSR.L.2	080625_o3_u2_hh_salt-r3-m120_07.mzxml	541.065	542.76996	547.065	549.76996
contamination_K1C9_HUMAN	4.1819196	0.86335444	R.SGGGGGGLGSGGSR.S.2	080517_o3_u2_hh_salt-r2-m120_09.mzxml	616.615	618.32	625.115	627.82
contamination_K1C9_HUMAN	-5.926555	2.5362816	K.TLNDRMQEYELQIAK.N.3	080625_o3_u2_hh_salt-r3-m120_11.mzxml	623.14	625.01	629.80664	632.01
contamination_K1C9_HUMAN	-3.972595	2.326805	K.SDLEM*QYETLQEELM*ALK.K.2	080625_o3_u2_hh_salt-r3-m120_11.mzxml	1101.855	1104.5599	1111.355	1115.0599
contamination_K1C9_HUMAN	2.1893399	3.365957	R.QGVADINDGLR.Q.2	080517_o3_u2_hh_salt-r2-m120_11.mzxml	579.12	580.825	586.12	588.825
contamination_K1C9_HUMAN	3.8510594	5.539256	R.GGSGGSFYSGGSGGGFASLSLGGFGGSGSR.G.3(3)	080723_o1_hh_salt-r4-m120_12.mzxml	902.20667	904.07666	912.8733	915.7433
contamination_K1C9_HUMAN	6.0686126	6.1900516	R.LASVLDKVALEEANNLLENK.I.3(3)	080723_o1_hh_salt-r4-m120_12.mzxml	792.89996	794.76996	800.89996	803.76996

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Ward/Euclidean Heatmap (HCA) (Jan 11, 2011, 18:59)

## Analysis Results

Accession	Alter
contamination_CAS1_BOVIN	
contamination_CAS2_BOVIN	
contamination_CASB_BOVIN	

Here, a quantification result has been selected. If a protein is chosen from the list, this protein is immediately propagated to other "listening" parts of the application, such as the protein overview page, where the corresponding protein will be highlighted. (Even if the view is changed, for example switched back to the search results or ms spectra view, the corresponding scan or hit will automatically be highlighted).

Please select a result from the following list for display and as input for further analysis:

Search protein by accession:

Map proteins on KEGG pathways...

Result(s)

Average Linkage/Pearson correlation (HCA) (Dec 23,2010 16:13) - 13 dataset(s)

Average Linkage/Euclidean (HCA) (Apr 22,2011 12:14) - 19 dataset(s)

Ward/Euclidean Heatmap (HCA) (Jan 11,2011 18:59)

Ward/Euclidean (HCA) (Jan 12,2011 15:56) - 23 dataset(s)

Neuralgas clustering (CA) (Jan 12,2011 16:03:01.107) - 14 dataset(s)

Comparison of clustering methods/Evaluation of cluster sizes (max K=50, 3/4 na) (CA) (Apr 28,2011 08:08:44.644)

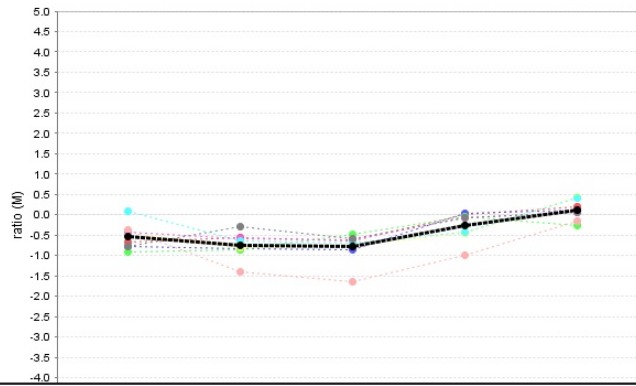
< Previous 2 of 6 Next >

Ward/Euclidean ... Quantification ... R:contamination... Ward/Euclidean ...

Treatment (factors and values) assigned to the following dataset:

HCA Cluster #16

Protein	Description	$\Delta$ COG	0min	10min	30min	60min
P94356	YxkC protein - Bacillus sub...		-0.6745	-0.554	-0.6371	0.0080
O31942	YonS protein - Bacillus sub...		-0.7814	-0.2983	-0.5859	-0.0687
O34563	Glutamine ABC transporter ...	ET	-0.3792	-1.4043	-1.6494	-0.9948
P02968	Flagellin - Bacillus subtil...	N	-0.7836	-0.8408	-0.851	0.0301
P28611	Chemotaxis protein motA - B...	N	-0.9107	-0.8737	-0.4911	-0.0379
P39214	Methyl-accepting chemotaxis...	NT	-0.4324	-0.7999	-0.74	-0.4571
P39215	Methyl-accepting chemotaxis...	NT	0.0834	-0.6531	-0.7074	-0.4376
P23447	Flagellar M-ring protein - ...	NU	-0.4374	-0.5811	-0.6068	-0.0683



Protein

- P94356
- P02968
- P28611
- P39214
- P23447
- P39215
- O34563
- O31942
- mean/prototype

hide all  show all

ns on ays...

ral) 08:49) -

ral) 10:10) -

ring of cluster

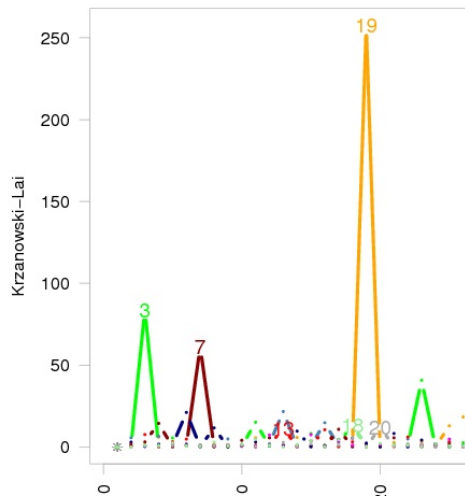
8,2011

CA) (Jan

ring (53) - 18

CA) (Jan

Next >



Here, the results of a hierarchical cluster analysis using Ward and Euclidean distances are shown. The resulting cluster tree has been 'cut' in 23 clusters. This was indicated as an optimal clustering by the cluster index of Krzanowski and Lai.



uni-bielefeld.de https://qupe.cebitec.uni-bielefeld.de/ProSE/app

Application Project Experiment Search Import Export Analyse Tools Settings Help

qupe user 1 qupe.evaluation Evaluation project Salt stress adaption P40780 Shapiro-Wilk test... (Dec 17,2010 11:29)

Please select a result from the following list for display and as input for further analysis:

Search protein by accession:

Map proteins on KEGG pathways...

Result(s)

- Quantification  $r > 0.6$ , exact 0.01 (Oct 15,2010 16:49) - 5 dataset(s)
- Average Linkage/Pearson correlation (HCA) (Dec 23,2010 16:36) - 92 dataset(s)
- Average Linkage/Uncentered pearson (HCA) (Dec 23,2010 16:49) - 66 dataset(s)
- Shapiro-Wilk test of normality (on residues) (Dec 17,2010 11:29) - 1 dataset(s)
- Map of expression values on KEGG pathways (Dec 18,2010 14:30) - 1 dataset(s)
- Average Linkage/Uncentered pearson (HCA) (Dec 23,2010 16:10) - 13 dataset(s)

< Previous 1 of 6 Next >

Analysis of Var... Fligner-Killeen... Shapiro-Wilk test...

Rename this result... Delete this result...

Treatment (factors and values) assigned to the following dataset:

Time

- 0min
- 10min
- 30min
- 60min
- 120min

Protein	Description	COG	Factors	Degrees of freedom	Mean Sq	Sum Sq	p-Value	Adjusted p-value	F
O32076	Uncharacterized protein yua...	S	Time, Residuals	4, 186	39.172337, 0.34149712	156.68995, 63.519467	0.0	0.0	114
P54466	UPF0365 protein yqfA - Bac...	S	Time, Residuals	4, 284	19.78543, 0.2496699	79.14172, 70.90625	4.2E-45	1.808E-42	79
P02968	Flagellin - Bacillus subtl...	N	Time, Residuals	4, 587	26.455494, 0.47451335	105.821976, 278.53934	7.34934E-40	2.944677E-37	55
P27206	Surfactin synthetase subuni...	Q	Time, Residuals	4, 257	39.795967, 0.7382535	159.18387, 189.73114	5.980888E-33	2.3923552E-30	53
O34992	Glycine betaine/carnitine/c...	E	Time, Residuals	4, 201	11.448162, 0.19587383	45.79265, 39.37064	1.16181865E-32	4.6395666E-30	58
P46920	Glycine betaine transport A...	E	Time, Residuals	4, 191	13.402711, 0.22718577	59.610844, 43.392483	2.3205078E-32	9.235621E-30	58
Q04747	Surfactin synthetase subuni...	Q	Time, Residuals	4, 388	41.24759, 1.0325946	164.59036, 400.64667	5.0550933E-28	2.006872E-25	39
O34538	Uncharacterized lipoprotein...	S	Time, Residuals	4, 225	6.078111, 0.14521676	24.312445, 32.67377	3.2619654E-26	1.29173835E-23	41
P40780	Uncharacterized protein ytx...	R	Time, Residuals	4, 88	10.303761, 0.15458286	41.215042, 13.6032915	7.9454033E-26	3.1384342E-23	66
P35136	D-3-phosphoglycerate dehydr...	HE	Time, Residuals	4, 220	16.395627, 0.46774659	65.34251, 102.904236	1.4263131E-22	5.619674E-20	34

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qupe.evaluation

Average Linkage/Pearson correlation (HCA) (Dec 23,2010 16:36) - 92 dataset(s)

Average Linkage/Uncentered pearson (HCA) (Dec 23,2010 16:49) - 66 dataset(s)

Shapiro-Wilk test of normality (on residues) (Dec 17,2010 11:29) - 1 dataset(s)

Map of expression values on KEGG pathways (Dec 18,2010 14:30) - 1 dataset(s)

Average Linkage/Uncentered pearson (HCA) (Dec 23,2010 16:10) - 13 dataset(s)

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Treatment (factors and values) assigned

Time

Protein	Description
P50865	Probable polysaccharide dea...
O31749	Uridylate kinase - Bacillus...
O34946	YcdI - Bacillus subtilis Pr...
Q01464	Septum site-determining pro...
O31620	YjbV protein - Bacillus sub...
P54470	UPF0085 protein yqfL - Bac...
P54382	Bifunctional protein fold - ...
P40780	Uncharacterized protein ytx...
P71013	Signal peptidase I T - Bac...
O31709	Uncharacterized protein ykn...

This page shows the results of an ANOVA sorted by an increasing adjusted p-value. Again, if a protein is selected in the tables, the same will be highlighted for example in a further open tab which shows the results of a Fligner-Killeen test of homogeneity of variances.

QuPE Application Project Experiment Search Import Export Analyse Tools Settings Help

qupe user 1 qupe.evaluation Evaluation project Salt stress

Quantification  $r > 0.6$ , exact 0.01 (Oct 15, 2010 16:49)

Please select a result from the following list for display and as input for further analysis:

Search protein by accession:

Map proteins on KEGG pathways...

Result(s)

- Quantification  $r > 0.6$ , exact 0.01 (Oct 15, 2010 16:49) - 5 dataset(s)
- Average Linkage/Pearson correlation (HCA) (Dec 23, 2010 16:36) - 92 dataset(s)
- Average Linkage/Uncentered pearson (HCA) (Dec 23, 2010 16:49) - 66 dataset(s)
- Shapiro-Wilk test of normality (on residues) (Dec 17, 2010 11:29) - 1 dataset(s)
- Map of expression values on KEGG pathways (Dec 18, 2010 14:30) - 1 dataset(s)
- Average Linkage/Uncentered pearson (HCA) (Dec 23, 2010 16:10) - 13 dataset(s)

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Protein quantification methods (SILAC, metabolic 15N)  
Data transformation, normalization & filtering  
Diagrams, plots & descriptive statistics  
Detect differently regulated proteins (inference statistics)  
Identify co-regulated proteins (cluster/ factor analysis)  
Special functions and extras

Protein statistics (Mean, median, one-sample t-test)  
Analysis of Variance (ANOVA)  
Kruskal-Wallis rank sum test  
Figner-Killeen test of homogeneity of variance  
Shapiro-Wilk test of normality (on residues)

When an analysis has been started the outcome is usually either one or more datasets of measurements or various kinds of illustrations.

Results have been produced using the following parameters:

- Enriched isotope: Nitrogen
- Incorporation level: 0.98
- Intensity threshold: 1.0
- Accuracy (m/z): 0.01
- Mass tolerance (da): 0.2
- Use exact peak positions: true
- Isotopic distribution similarity: 0.8
- Elution peak interval (seconds before): 30
- Elution peak interval (seconds after): 30
- Maximal allowed peak width (seconds between): 180
- Peak shift optimisation: false
- Maximal peak shift: 3
- Smoothing filter: Filter turned off
- Peak detection method: CWT-based peak detection (6-point overlap, skip non-overlapping)
- Signal/Noise computation method: Sliding window (20-point)
- Filter threshold: 0.6

Rename this result... Delete this result...

Treatment (factors and values) assigned to the following dataset:

Time 0min

Protein/Peptide	Ratio(M)	Intensity (A)	Peptide(s)	Sample	Unlabeled Start	Labeled Stop	Labeled Start	Labeled Stop
contamination_K1C9_HUMAN -3.4937372	2.408694		K.EIETYHNLLEGGQEDFESSGAGK.I.3	080621_o3_u2_hh_salt-r3-m000_05.mzxml	837.2033	839.0733	845.5366	848.4067
contamination_K1C9_HUMAN -3.9491735	3.4646528		K.DIENQYETQITQIEHEVSSSGQEVQSSAK.E.4	080621_o3_u2_hh_salt-r3-m000_10.mzxml	816.70496	818.4075	825.45496	827.9075
contamination_K1C9_HUMAN -3.656885	2.8874717		K.DIENQYETQITQIEHEVSSSGQEVQSSAK.E.4	080621_o3_u2_hh_salt-r3-m000_12.mzxml	816.70496	818.4075	825.45496	827.9075
contamination_K1C9_HUMAN -3.4945233	1.9975523		K.DIENQYETQITQIEHEVSSSGQEVQSSAK.E.4	080621_o3_u2_hh_salt-r3-m000_03.mzxml	816.70496	818.4075	825.45496	827.9075
contamination_K1C9_HUMAN -3.765317	2.1697242		K.DIENQYETQITQIEHEVSSSGQEVQSSAK.E.4	080621_o3_u2_hh_salt-r3-m000_02.mzxml	816.70496	818.4075	825.45496	827.9075
contamination_K1C9_HUMAN -2.9910243	1.4855258		K.DIENQYETQITQIEHEVSSSGQEVQSSAK.E.4	080621_o3_u2_hh_salt-r3-m000_01.mzxml	816.70496	818.4075	825.45496	827.9075

Analyse Tools Settings Help

Protein quantification methods (SILAC, Data transformation, normalization & filtering)

Diagrams, plots & descriptive statistics

Detect differently regulated proteins (inference statistics)

Identify co-regulated proteins (cluster/ factor analysis)

Special functions and extras

When an analysis has been started the outcome is usually either one or more datasets of measurements or various kinds of illustrations.

To perform a new analysis, e. g. an Analysis of Variance, simply select the appropriate function from the "Analyse" menu. This is, of course, only possible if you have write access to the current experiment.

Further information on how to set up a new experiment, import data, perform MIS/PMF database searches or to conduct analyses can be found online in the QuPE documentation (e. g. select the "Documentation" entry from the "Help" menu).

Thank you very much for  
your interest in QuPE

[QuPE@CeBiTec.Uni-Bielefeld.de](mailto:QuPE@CeBiTec.Uni-Bielefeld.de)

If you have further questions please do not hesitate to contact us.