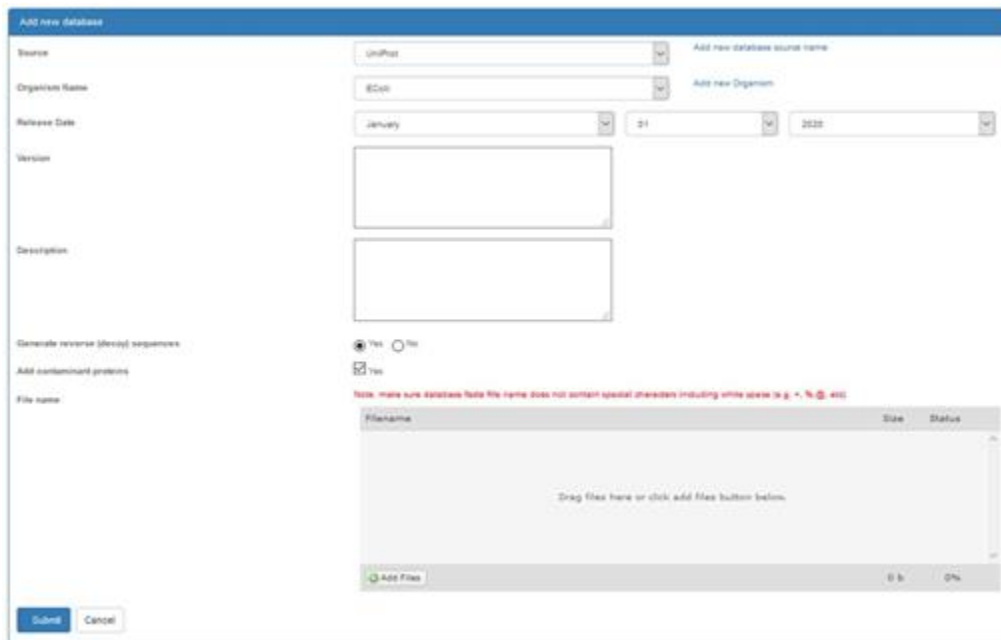


# Common Tasks User Guide

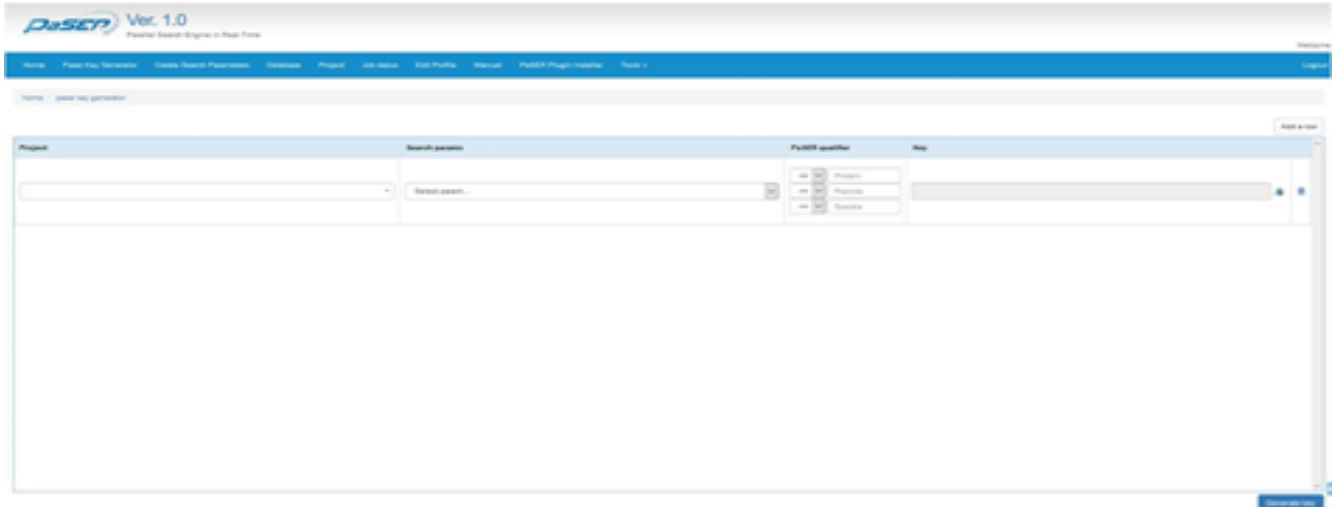
## Add new database:

- Log into PDV and navigate to the Database tab.
- Add the source, species and release data for the FASTA file
- Additional fields you would like captured can be entered in the “Version” box
  - Source, species, release date and version fields will be used to autogenerate a FASTA filename in PDV
- Click on add files to upload your FASTA sequence
- Click on “Submit” to save your FASTA file in PDV
- 



## Create new search parameters:

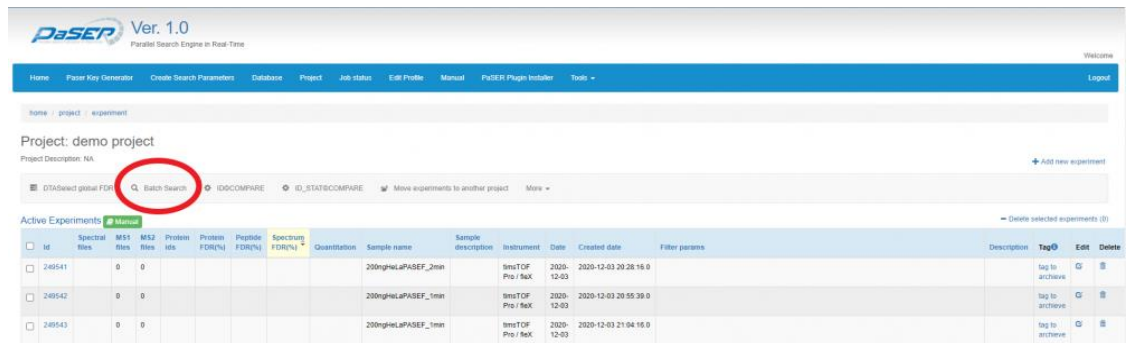
- Log into PDV and navigate to the “Create Search Parameter” tab.
- Create search parameters as desired.
  - Select a FASTA file and click “Add Database”
  - Select desired FDR filter in the Basic DTAselct 2.0 Parameters section
- Press Save at the bottom left of the page
- Enter a name for your search parameters



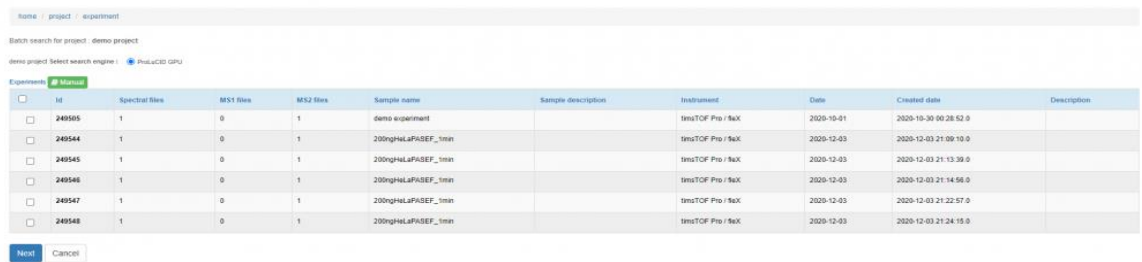
### Perform an offline Search:

Note: Real-time search task have priority over offline searches. Any offline searches that are queued will be cancelled, the queue cleared when a real-time search task is requested.

- Navigate to the projects tab, and select the project.
- Click on the desired experiment
- Click the batch search link



- Select the experiments you wish to search



- Select your search engine parameter s and submit you search

ProLuCID Batch Search

Basic parameters

Search Name

User

Protein database  Add Database

Fragmentation/activation method  CID/HCD  ETD

Precursor mass type  mono  average

Fragment mass type  mono  average

Precursor/peptide mass tolerance  High resolution (e.g. OrbiTrap)  
   
ppm precursor tolerance      number of isotopic peaks  
 Low resolution (e.g. LTQ)  
  
milli-amu precursor tolerance

precursor mass range Start  End

precursor charge range Start  End

Fragment mass tolerance in ppm

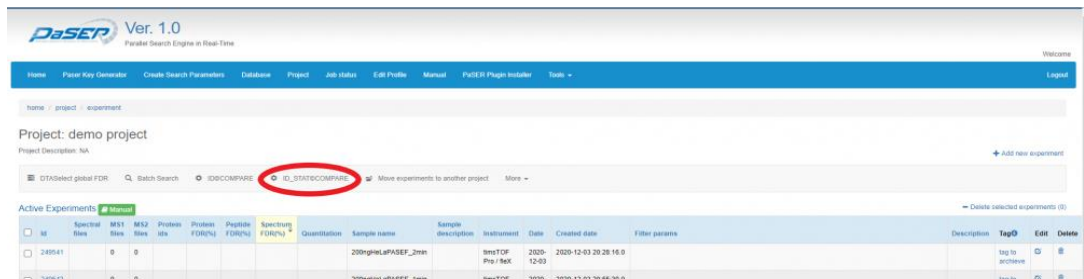
Use low fragment ions  yes  no

Enzyme information

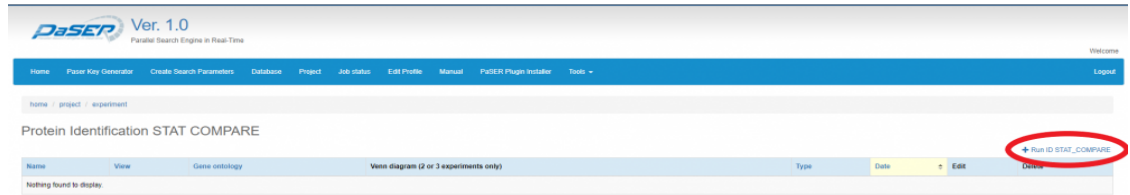
Specificity  none  one end  both end

IDstatCompare for comparing multiple experiments:

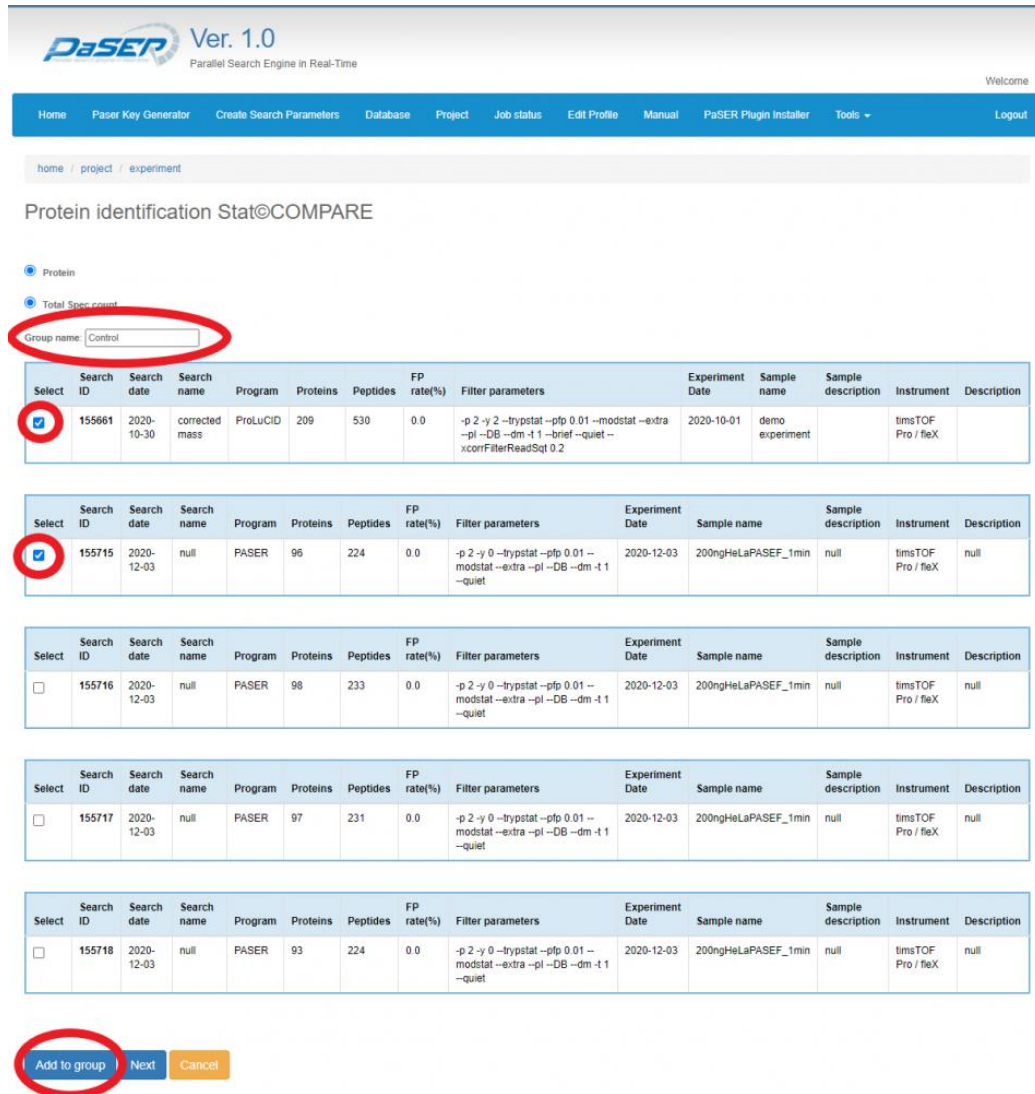
- Log into PDV and select the projects tab from the navbar.
- Click view on the desired project to see the list of experiments
- Click “Identification STAT COMPARE” to list all existing comparisons.



- Click “ID@Stat\_COMPARE” to build a new comparison.



- 
- Create a group name, such as “control”, and select experiments by clicking checkboxes. Then, click on “Add to group” to add selected experiments to a group.



- 
- Create another group name, for example, “mutant,” and select experiments by clicking checkboxes as before. Then, click on “Add to group” to add them to this group.

Protein identification Stat@COMPARE

Group name: control

Group name: mutant

Select	Search ID	Search date	Search name	Program	Proteins	Peptides	FP rate(%)	Filter parameters	Experiment Date	Sample name	Sample description	Instrument	Description
<input type="checkbox"/>	155681	2020-10-30	corrected mass	PROLUCID	209	530	0.0	-p 2 -y 2 -trypstat -pfp 0.01 -modstat -extra -pi -DB -dm -1 -brief -quiet --vcconf useReadlist 0.2	2020-10-01	demo experiment		imsTOF Pro / S&X	
<input type="checkbox"/>	155715	2020-12-03	null	PaSER	96	224	0.0	-p 2 -y 0 -trypstat -pfp 0.01 -modstat -extra -pi -DB -dm -1 -quiet	2020-12-03	200ngHeLaPaSEF_1min	null	imsTOF Pro / S&X	null
<input checked="" type="checkbox"/>	155716	2020-12-03	null	PaSER	98	233	0.0	-p 2 -y 0 -trypstat -pfp 0.01 -modstat -extra -pi -DB -dm -1 -quiet	2020-12-03	200ngHeLaPaSEF_1min	null	imsTOF Pro / S&X	null
<input checked="" type="checkbox"/>	155717	2020-12-03	null	PaSER	97	231	0.0	-p 2 -y 0 -trypstat -pfp 0.01 -modstat -extra -pi -DB -dm -1 -quiet	2020-12-03	200ngHeLaPaSEF_1min	null	imsTOF Pro / S&X	null
<input type="checkbox"/>	155718	2020-12-03	null	PaSER	93	224	0.0	-p 2 -y 0 -trypstat -pfp 0.01 -modstat -extra -pi -DB -dm -1 -quiet	2020-12-03	200ngHeLaPaSEF_1min	null	imsTOF Pro / S&X	null

Buttons: Add to group, Next, Cancel

- Verify groups and selected experiments and click on the “Next” button.
- Name the comparison, for example, “My comparison,” and click the run button.
- Click “view” to open comparison results.

IDStat COMPARE

Sample information

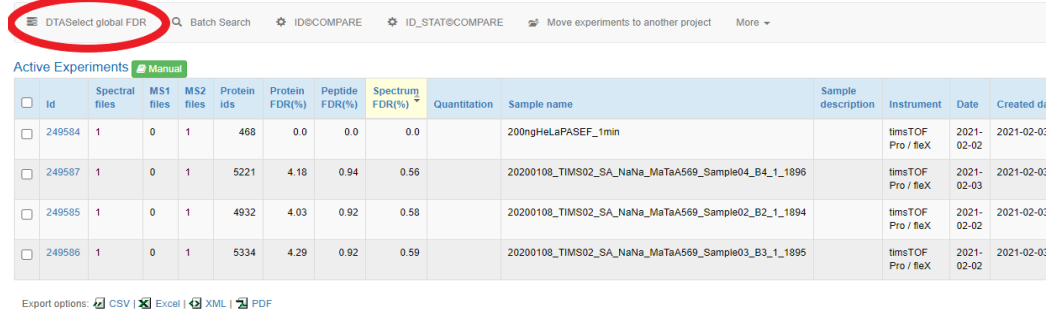
group index	group name	sample
1	control	demo experiment.200ngHeLaPaSEF_1min.
2	mutant	200ngHeLaPaSEF_1min.200ngHeLaPaSEF_1min.

Export options: CSV, Excel, HTML, PDF

accession	1 best p-value	q-value	norm spec count 1	norm spec count 2	norm spec count Average 1	norm spec count Average 2	avg ratio change 1/2	NSAF-1	NSAF-2	NSAF average 1	NSAF average 2	EMPA1.1	EMPA1.2
Q9Y286	0.50337676811827	0.547982929	0.02807	2.5552831	1.3037330319742082	2.583355455891645	0.5027205309743522	0.00105802715	0.010480240105297255	0.0052601357	0.01022139	0.002310483	0.23310
F5H92	0.296757682718768	0.547982929	0.01738	2.5552831	0.8691553544494721	2.583355455891645	0.33514702064956814	0.0019568215	0.022546518010287611	0.007834608	0.022710465	0.002618276	0.51705
Reverse_Revista_ssd[272627]H4N1_H4N1AAN	0.4999999999999999	0.547982929	0.01738	0.00000	0.8691553544494721	0.0	100000.0	0.0	0.0	0.0	0.0	2.6688538E-4	0.0
Q71U9	0.4999999999999999	0.547982929	24.28000	0.00000	*2.141410048822385	0.0	100000.0	0.0	0.0	0.0	0.0	0.0	0.0
F5H7A5	0.296757682718768	0.547982929	0.01738	2.5552831	0.8691553544494721	2.583355455891645	0.33514702064956814	0.0015159955	0.0221008340102428267	0.0076799775	0.0226223	0.002560296	0.50805
G3V1L6	0.50337676811827	0.547982929	0.01738	1.7041754	0.8691553544494721	1.7289030371081985	0.5027205309743522	0.005598841	0.005322055010054101455	0.0027784200	0.005372095	0.00496478224	0.09647

## Combining Multiple Experiments/fractions into single analysis:

- Log into PDV and select the projects tab from the navbar.
- Click view on the desired project to see the list of experiments
- Click “DTASelect global FDR”



DTASelect global FDR

Active Experiments Manual

<input type="checkbox"/>	ID	Spectral files	MS1 files	MS2 files	Protein ids	Protein FDR(%)	Peptide FDR(%)	Spectrum FDR(%)	Quantitation	Sample name	Sample description	Instrument	Date	Created date
<input type="checkbox"/>	249584	1	0	1	468	0.0	0.0	0.0		200ngHeLaPASEF_1min		timsTOF Pro / feX	2021-02-02	2021-02-01
<input type="checkbox"/>	249587	1	0	1	5221	4.18	0.94	0.56		20200108_TIMS02_SA_NaNa_MaTaA569_Sample04_B4_1_1896		timsTOF Pro / feX	2021-02-03	2021-02-01
<input type="checkbox"/>	249585	1	0	1	4932	4.03	0.92	0.58		20200108_TIMS02_SA_NaNa_MaTaA569_Sample02_B2_1_1894		timsTOF Pro / feX	2021-02-02	2021-02-01
<input type="checkbox"/>	249586	1	0	1	5334	4.29	0.92	0.59		20200108_TIMS02_SA_NaNa_MaTaA569_Sample03_B3_1_1895		timsTOF Pro / feX	2021-02-02	2021-02-01

Export options: [CSV](#) | [Excel](#) | [XML](#) | [PDF](#)

- Select the experiments you wish to combine and click next
- Enter an experiment name, then fill in your desired parameters and click run.
- You will see a new experiment in your project with the name you created.
- You can click the experiment to view it more in depth.

### Select search results to Combine Multiple DTA Select

<input type="checkbox"/>	Experiment ID	Search id	searched date	sampleName	Home Folder	start date	description
<input type="checkbox"/>	249588	188780	2021-02-08	CombiningTest	home\p1\p2_data\paser\PaSER_phospho_search_west\CombiningTest_2021_02_08_18_249588		
<input type="checkbox"/>	249587	188780	2021-02-03	20200108_TIMS02_SA_NaNa_MaTaA569_Sample04_B4_1_1896	home\p1\p2_data\paser\PaSER_phospho_search_west\20200108_TIMS02_SA_NaNa_MaTaA569_Sample04_B4_1_1896_2021_02_03_11_249587		
<input type="checkbox"/>	249588	188780	2021-02-03	20200108_TIMS02_SA_NaNa_MaTaA569_Sample03_B3_1_1895	home\p1\p2_data\paser\PaSER_phospho_search_west\20200108_TIMS02_SA_NaNa_MaTaA569_Sample03_B3_1_1895_2021_02_03_02_249588		
<input type="checkbox"/>	249589	188787	2021-02-03	20200108_TIMS02_SA_NaNa_MaTaA569_Sample02_B2_1_1894	home\p1\p2_data\paser\PaSER_phospho_search_west\20200108_TIMS02_SA_NaNa_MaTaA569_Sample02_B2_1_1894_2021_02_03_01_249589		
<input type="checkbox"/>	249584	188780	2021-02-03	200ngHeLaPASEF_1min	home\p1\p2_data\paser\PaSER_phospho_search_west\200ngHeLaPASEF_1min_2021_02_03_01_249584		