

Shotgun
Protein
Sequencing

Project Status

Create Project Run Project Project Status Reports

Project	abrf_olc 1. Name of the project
User	pbouchard 2. Username executing the job
Status	100 % 3. Percentage of completion
Elapsed	1:13 4. Elapsed and remaining time
Data	Group by Contig 5. All spectra sorted by contig Group by Protein 6. All contig sorted by protein with statistics
Cluster Data	All Clusters (txt) Group by ABRF_Ab_LC_DTT_NIPIA_ArgC_37C_On_102909.mgf 7. All spectra sorted by input Group by ABRF_Ab_LC_DTT_NIPIA_AspN_37C_ON_102909.mgf Group by ABRF_Ab_LC_DTT_NIPIA_GluC_37C_ON_102909.mgf Group by ABRF_Ab_LC_DTT_NIPIA_LysC_37C_ON_102909.mgf Group by ABRF_Ab_LC_DTT_NIPIA_chymotrypsin_37C_ON_102909.mgf Group by ABRF_Ab_LC_DTT_NIPIA_pepsin_37C_1h_102809.mgf Group by ABRF_Ab_LC_DTT_NIPIA_trypsin_37C_ON_102909.mgf

Project
abrf_olc
aHerceptin_gtabOboth
aMRSA_HC
▼ Next ▼

Protein
gi|124487419
gi|71043961
gi|22507367
▼ Next ▼

Contig
18
19
20
▼ Next ▼

Input File
Ab_LC_DTT_NIPIA_ArgC
Ab_LC_DTT_NIPIA_AspN
Ab_LC_DTT_NIPIA_GluC
▼ Next ▼

Shotgun Protein Sequencing



The screenshot shows a software interface titled "Proteins". At the top, there is a navigation bar with four tabs: "Create Project", "Run Project", "Project Status", and "Reports". On the left side, there is a sidebar with several sections: "Project" (listing "abrf_olc", "aHerceptin_gtabOboth", and "aMRSA_HC" with a "Next" button), "Protein" (listing "gi|124487419", "gi|71043961", and "gi|22507367" with a "Next" button), "Contig" (listing "18", "19", and "20" with a "Next" button), and "Input File" (listing "Ab_LC_DTT_NIPIA_ArgC", "Ab_LC_DTT_NIPIA_AspN", and "Ab_LC_DTT_NIPIA_GluC" with a "Next" button). The main content area displays a table of protein results:

Protein	Description	Contigs	Spectra	Amino Acids	Coverage (%)
gi 124487419/ref NP_034798.2/	keratin complex 2, basic, gene 17 [Mus musculus]	9	27	71	100
gi 71043961/ref NP_075822.3/	trypsinogen 7 [Mus musculus]	4	375	35	141
gi 22507367/ref NP_683761.1/	oxysterol-binding protein-like protein 10 [Mus musculus]	2	5	17	28
gi 16716569/ref NP_444473.1/	protease, serine, 1 [Mus musculus]	5	18	48	195
gi 31980626/ref NP_058038.2/	regulator of G-protein signaling 14 [Mus musculus]	2	5	13	23
gi 121040/sp P01868.1/IGHG1_MOUSE	Ig gamma-1 chain C region secreted form	2	15	11	33
gi 3212688/pdb 2JEL/L	Chain L, Jel42 FabHPR COMPLEX	50	272	141	649
gi 148667160/gb EDK99576.1/	hypothetical protein C630010N09 [Mus musculus]	2	6	16	118
gi 6978717/ref NP_036668.1/	Chymotrypsinogen B [Rattus norvegicus]	1	4	12	45
gi 149044187/gb EDL97569.1/	echinoderm microtubule associated protein like 1, isoform CRA_b [Rattus norvegicus]	4	11	22	35



Protein

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Project

[abrf_olc](#)
[aHerceptin_gtabOboth](#)
[aMRSA_HC](#)

▼ Next ▼

Protein

[gi|124487419](#)
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▼ Next ▼

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18
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20

▼ Next ▼

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[Ab_LC_DTT_NIPIA_GluC](#)

▼ Next ▼

GI 71043961 REF NP_075822.3 1. Name of the protein

4 contigs, 375 spectra, 35 amino acids, 14.1% coverage 2. General statistics

```

1 MKTLIFLAFL GAAVALPLDD DDDKIVGGYT CQRNALPYQV SLNSGYHFCG
51 GSLINSQWVV SAAHCYKSRI QVRLGEHNID ALEGGEQFID AAKIIRHPNY
101 NANTYNNDIM LIKLKTAATL NSRVSTVALP RSCPSAGTRC LVSGWGNTLS
151 SGTNYPSSLQ CLDAPVLSDS SCTSSYPGKI TSNMFCLGFL EGGKDSCQGD
201 SGGPVVCNGQ LQGVVSWGYG CAQRGKPGVY TKVCKYVNWI QQTIAAN

```

3. Common amino acids

Index	Spectra	Contig	Contig Sequence	Protein
18	2	 Homolog TAA(T,55.0)LNS De Novo [243.1]RINS	<code>gi 71043961 ref NP_075822.3 </code> trypsinogen 7 [Mus musculus]	
23	5	 Homolog (P,4.0)L(DDDDKIVG,-368.2) De Novo [275.2]TID[229.1]IFI[255.2]	<code>gi 71043961 ref NP_075822.3 </code> trypsinogen 7 [Mus musculus]	



- Project
 - [abrf_olc](#)
 - [aHerceptin_gtabOboth](#)
 - [aMRSA_HC](#)
- ▼ Next ▼

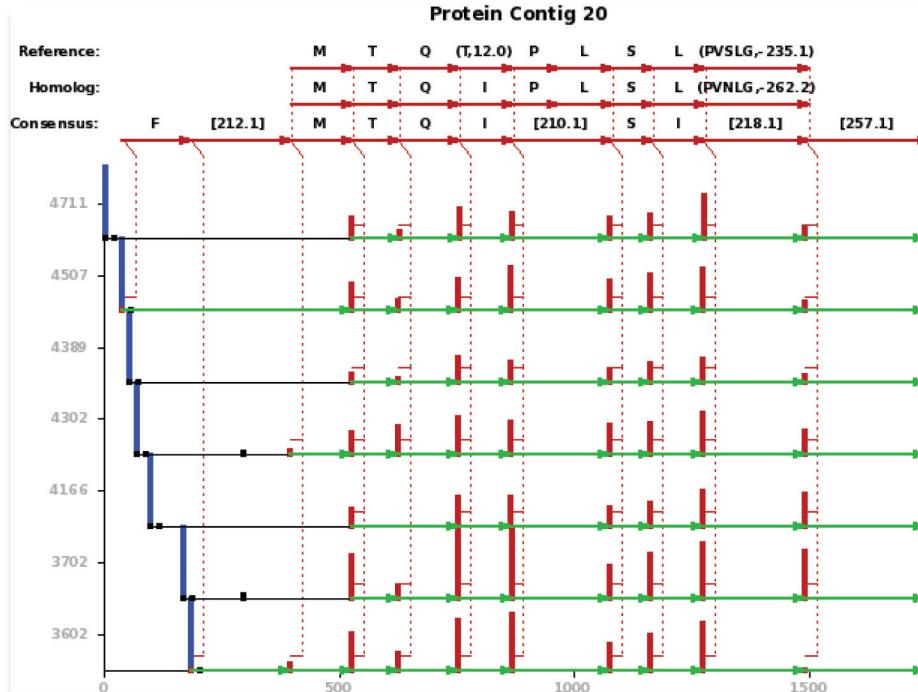
- Protein
 - [gi|124487419](#)
 - [gi|71043961](#)
 - [gi|22507367](#)
- ▼ Next ▼

- Contig
 - [18](#)
 - [19](#)
 - 20**
- ▼ Next ▼

- Input File
 - [Ab_LC_DTT_NIPIA_ArgC](#)
 - [Ab_LC_DTT_NIPIA_AspN](#)
 - [Ab_LC_DTT_NIPIA_GluC](#)
- ▼ Next ▼

Create Project Run Project Project Status Reports

2. Reference peptide



1. Contig index

3. Database peptide

4. De Novo peptide

5. Spectra alignment

Index	Spectrum	Peptide	Mass (m)	Charge (z)	B (%)	Y (%)	BY Intensity (%)
3602	<p>Reference</p> <p>M T Q (T) P L S L (PVSLG,-235.1)</p> <p>(PVSLG,-235.1) S L P(T) Q I T M</p>	<p>Reference 2.</p> <p>[212.1]MTQ(T,12.0)PLS(PVSLG,-235.1)[257.1]</p> <p>Homolog 3.</p> <p>[212.1]MTQIPLS(PVNLG,-262.1)[257.1]</p> <p>De Novo 4.</p> <p>[212.1]MTQI[210.1]SI[218.1][257.1]</p>	795.5	0	81	109	46

6. Link to associated cluster



Cluster

Create Project Run Project Project Status Reports

Project

- [abrf_olc](#)
- [aHerceptin_gtabOboth](#)
- [aMRSA_HC](#)

▼ Next ▼

Protein

- [gi|124487419](#)
- [gi|71043961](#)
- [gi|22507367](#)

▼ Next ▼

Contig

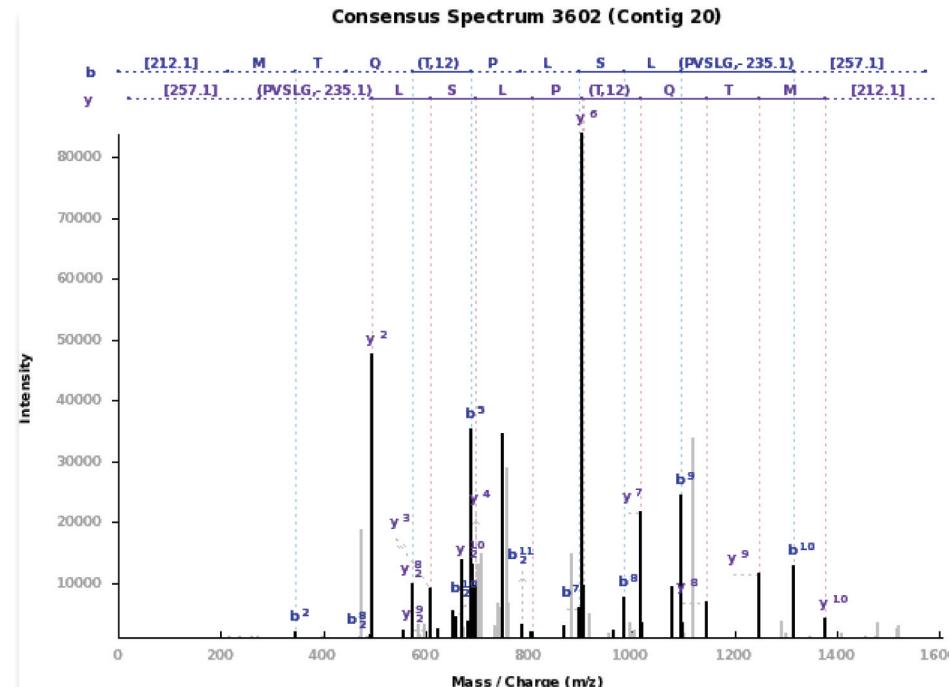
- [18](#)
- [19](#)
- [20](#)

▼ Next ▼

Input File

- [Ab_LC_DTT_NIPIA_ArgC](#)
- [Ab_LC_DTT_NIPIA_AspN](#)
- [Ab_LC_DTT_NIPIA_GluC](#)

▼ Next ▼



1. Consensus spectrum of the cluster

Scan	Spectrum	Peptide	Mass (m)	Charge (z)	B (%)	Y (%)	BY Intensity (%)
3235	<p>Reference</p> <p>M, T, Q, (T), P, L, S, (PVS, L, G)</p> <p>b: [212.1], M, T, Q, (T,12.0), P, L, S, (PVS, L, G), (PVS, L, G, -235.1), [257.1]</p> <p>y: [257.1], (PVSLG, -235.1), L, S, L, P, (T,12), Q, T, M, [212.1]</p> <p>50000</p> <p>0 1000</p>	<p>Reference</p> <p>[212.1]MTQ(T,12.0)PLS(PVSLG,-235.1)[257.1]</p> <p>Homolog</p> <p>[212.1]MTQIPLSL(PVNLG,-262.1)[257.1]</p> <p>De Novo</p> <p>[212.1]MTQI[210.1]SI[218.1][257.1]</p>	1589.9	2	81	109	45

ABRF_Ab_LC_DTT_NIPIA_AspN_37C_ON_102909.mgf

2. Input filename



Create Project Run Project Project Status Reports

- Project
 - abrf_olc
 - aHerceptin_gtabOboth
 - aMRSA_HC

▼ Next ▼

- Protein
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▼ Next ▼

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 - 18
 - 19
 - 20

▼ Next ▼

- Input File
 - Ab_LC_DTT_NIPIA_ArgC
 - Ab_LC_DTT_NIPIA_AspN
 - Ab_LC_DTT_NIPIA_GluC

▼ Next ▼

ABRF_Ab_LC_DTT_NIPIA_ArgC_37C_On_102909.mgf 1. Input filename

2. Pagination

[40-1205] [1258-1556] [1583-1790] [1795-1914] [1920-2130] [2140-2420] [2432-2693]

Scan	Spectrum	Peptide	Mass (m)	Charge (z)	B (%)	Y (%)	BY Intensity (%)
620 (54)	<p>Homolog</p> <p>100000 50000 0 500 1000</p>	<p>Homolog <u>HNSY(TCE,-91.0)ATHK</u> De Novo <u>[251.1]SY[299.1]ATHQ</u></p>	1256.6	2	111	111	55
633 (54)	<p>Homolog</p> <p>30000 20000 0 500 1000</p>	<p>Homolog <u>[12.0]HNSY(TCE,-91.0)ATHK</u> De Novo <u>[12.0][251.1]SY[299.1]ATHQ</u></p>	1268.6	2	80	40	44

gi/3212688/pdb/2JEL/L

3. Protein name

SPS projects:

Description:

Database:

Parent mass tolerance: Peak mass tolerance:

Per SPS project (get these from SPS params file)

Parent mass tolerance: MS/MS type:

Peak mass tolerance: Cysteine-protecting group:

Advanced parameters

Tag length: CLUSTALW min score:
Maximum aa jump: Smallest reported sequence:
Double aa jumps: Grid # nodes:
Match flanking masses: Grid path:
Minimum modification mass: Maximum modification mass:

Spectrum files: One or more spectrum files (MGF,mzXML)

Description: Project name and info

Parent mass tolerance: 0-3 Da Enable correction

MS/MS type: <dropdown>

Peak mass tolerance: 0-0.4 Da

Cysteine-protecting group: <dropdown>

Discard low quality spectra

Minimum quality: 0.15 (0-1)

MS-Cluster

Minimum cluster size: 3

Advanced parameters

Minimum spectrum overlap: 0.45 Filter triangles

Minimum # matched peaks: 4

Min spectra per contig: 1

Minimum % matched score: 0.4

Smallest reported sequence: 4

Maximum alignment p-value: 0.05

Grid # nodes: 64

Maximum modification mass: 100 Da

Grid path: ~nbandeir