SBEAMS – Proteomics & PeptideAtlas
Proteomics Analysis Database

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Day 5

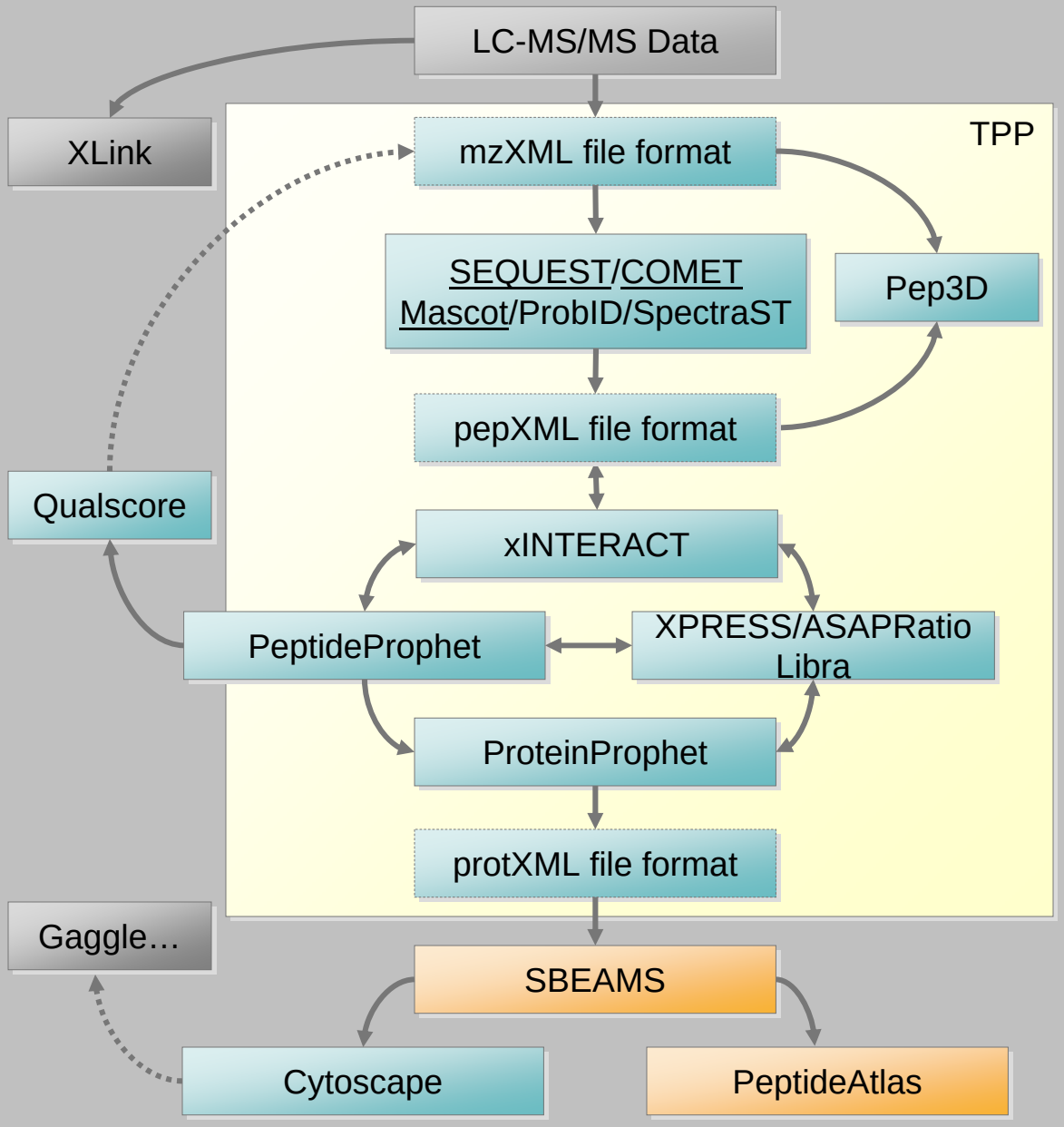
October 20, 2006

INSTITUTE FOR Systems Biology

Outline

Topics

- Introduction to SBEAMS
- SBEAMS – Proteomics
- PeptideAtlas
- Tutorial and Exercises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Pep3D
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Qualscore
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PeptideProphet
XPRESS/ASAPRatio
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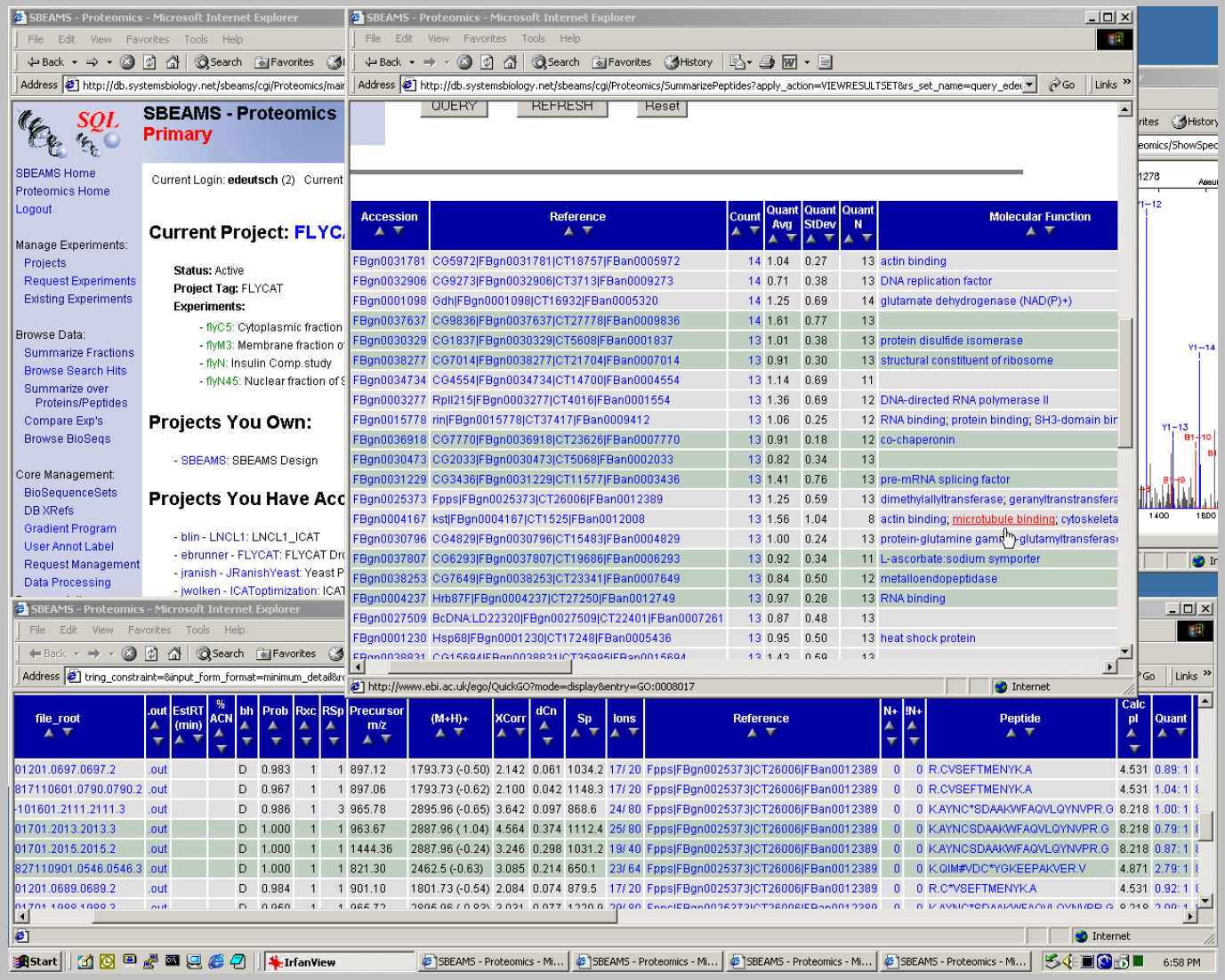
ProteinProphet
protXML file format
Gaggle…
SBEAMS
Cytoscape
PeptideAtlas

SBEAMS
Systems Biology Experiment Analysis Management System

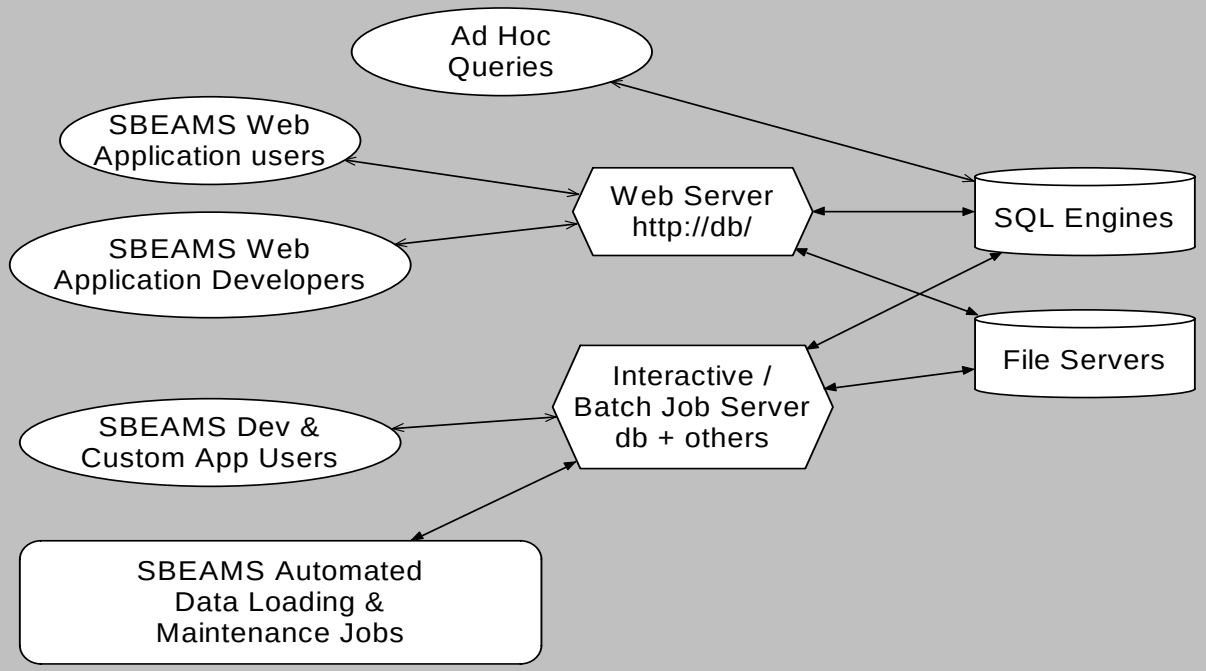


A Need for Custom Database Front End Software

- Many databases for many Data Types
  - Many data types are generated and used at ISB, even as part of one project (Proteomics, Microarray, Genotyping, Immunostain, Interactions, ...)
  - Relational Database needed to keep track of it all
  - One grand unified database tough
  - Allow different databases to evolve under a common system using common software, database engines, interface
  - Integration of different data types relatively easy to integrate in this model
- Data Accessibility
  - Making data available to all levels of users
  - Reasonably simple web interface for data entry and queries
  - Client platform independence
  - UNIX command line interface for maintenance jobs and complex data mining
  - Remote data access via HTTP for scripting and automation
  - Relational back-end, flavor independent

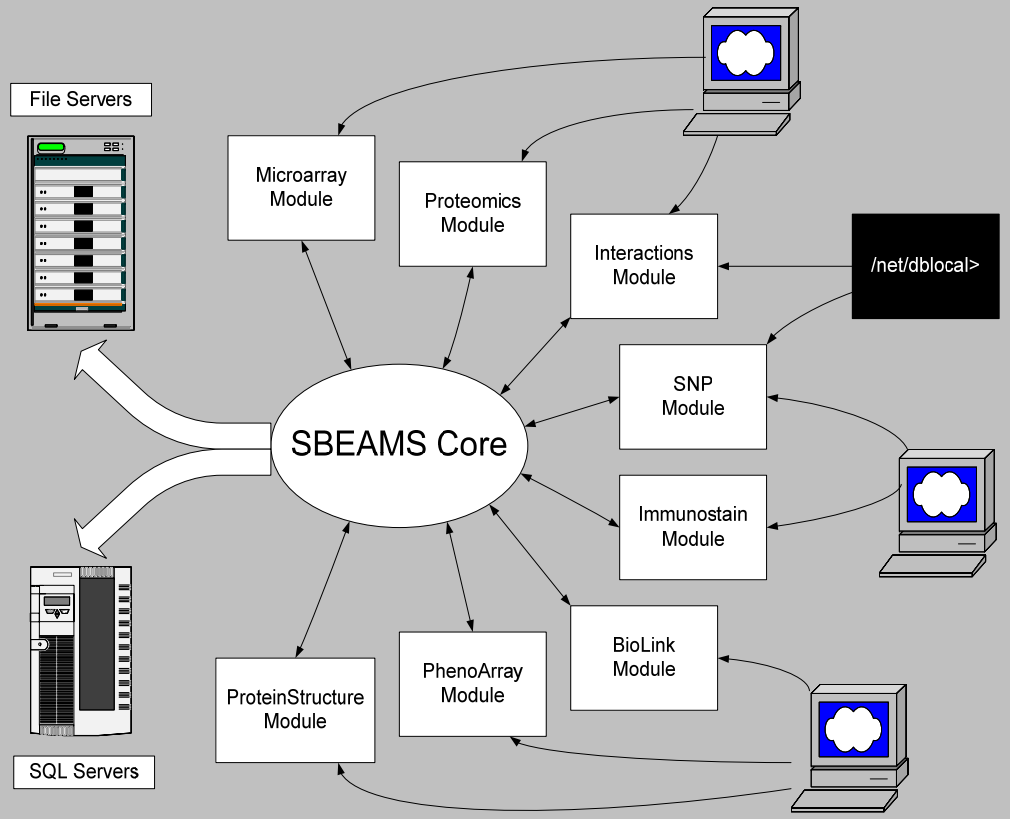
SBEAMS
Systems Biology Experiment Analysis Management System

- A framework for writing software for collecting, storing, accessing, and integrating data produced by various experiments using a relational database
- Tools for creating web front end entering data, queries, triggering batch jobs
- Programming interface for maintenance jobs, data loading and retrieval scripts, and interactive applications



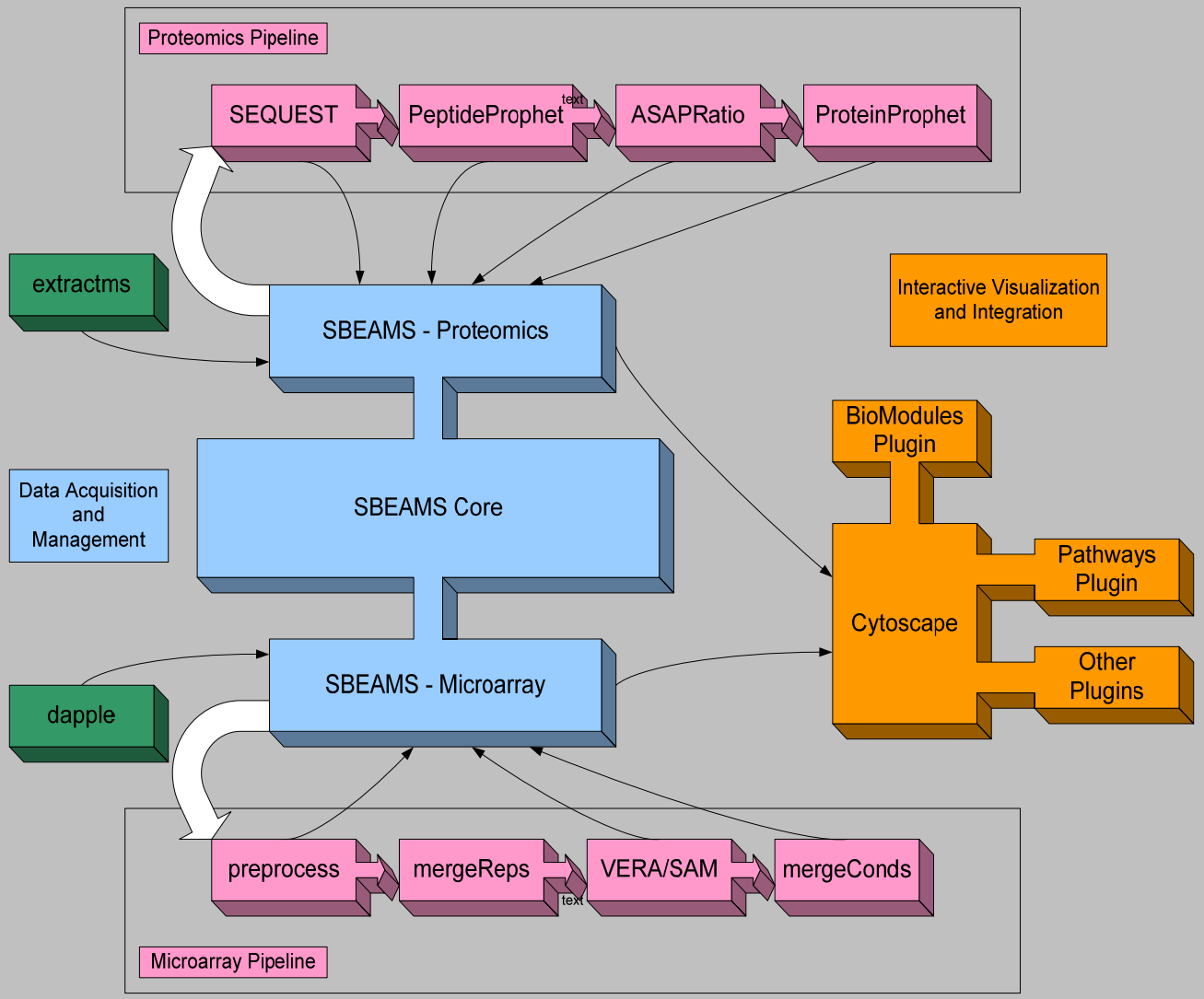
SBEAMS
Systems Biology Experiment Analysis Management System

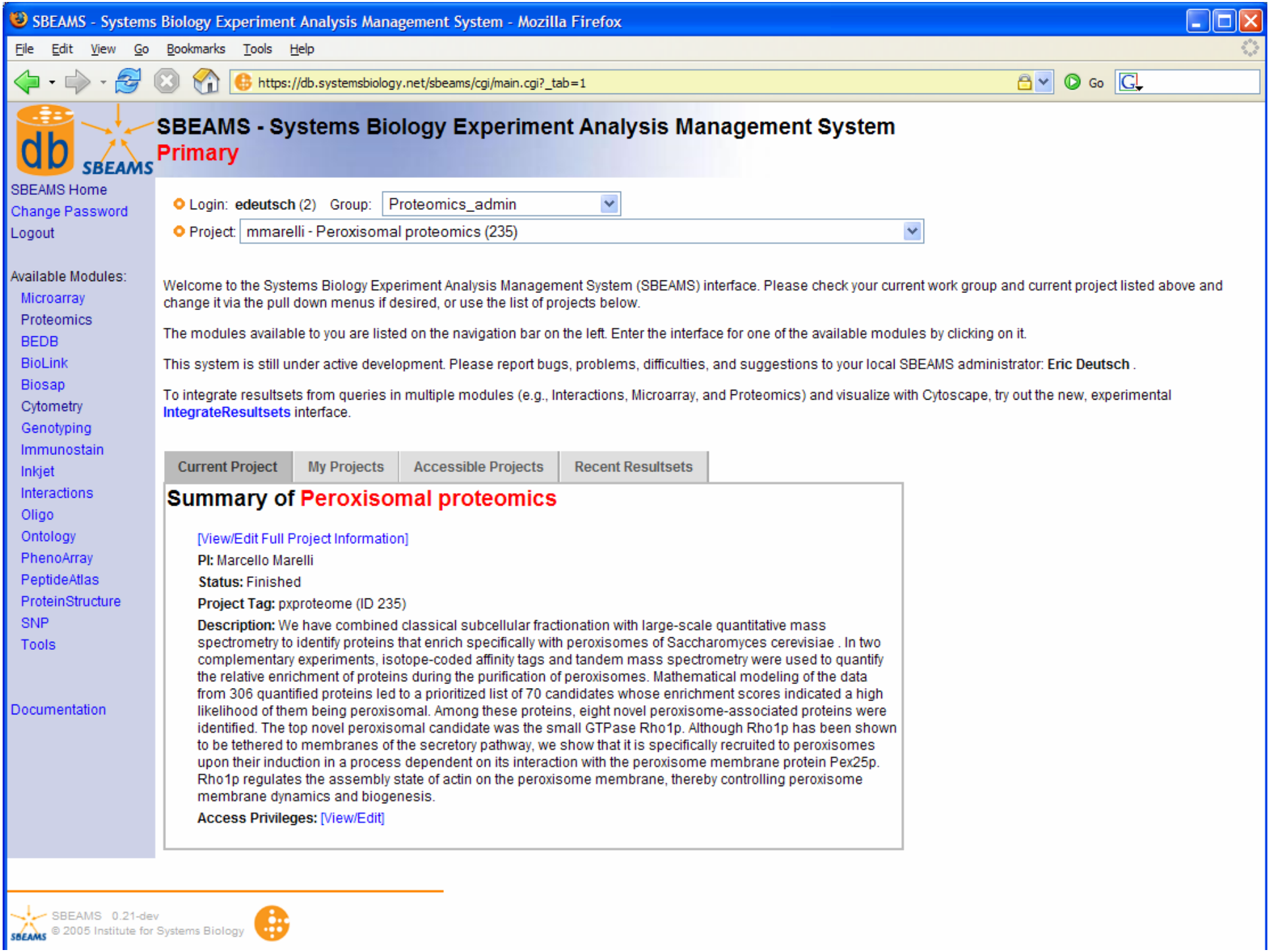
- SBEAMS is designed as a core set of functionality around which individual modules can be built
- Each experiment or data type can have its own module
- Simultaneous “live” and development environments allow continual development
- Web interface accessible from any platform with a browser / no client installation
- Also UNIX command-line client and scriptable HTTP client API



SBEAMS

Integration of data acquisition, management, and analysis tools




SBEAMS - Systems Biology Experiment Analysis Management System - Mozilla Firefox
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Go
SBEAMS - Systems Biology Experiment Analysis Management System
Primary
SBEAMS Home
Change Password
Logout
Available Modules:
Microarray
Proteomics
BEDB
BioLink
Biosap
Cytometry
Genotyping
Immunostain
Inkjet
Interactions
Oligo
Ontology
PhenoArray
PeptideAtlas
ProteinStructure
SNP
Tools
Documentation
Login: edeutsch (2) Group: Proteomics_admin
Project: mmarelli - Peroxisomal proteomics (235)
Welcome to the Systems Biology Experiment Analysis Management System (SBEAMS) interface. Please check your current work group and current project listed above and change it via the pull down menus if desired, or use the list of projects below.
The modules available to you are listed on the navigation bar on the left. Enter the interface for one of the available modules by clicking on it.
This system is still under active development. Please report bugs, problems, difficulties, and suggestions to your local SBEAMS administrator: Eric Deutsch .
To integrate resultsets from queries in multiple modules (e.g., Interactions, Microarray, and Proteomics) and visualize with Cytoscape, try out the new, experimental IntegrateResultsets interface.
Current Project
My Projects
Accessible Projects
Recent Resultsets
Summary of Peroxisomal proteomics
[View/Edit Full Project Information]
PI: Marcello Marelli
Status: Finished
Project Tag: pxproteome (ID 235)
Description: We have combined classical subcellular fractionation with large-scale quantitative mass spectrometry to identify proteins that enrich specifically with peroxisomes of Saccharomyces cerevisiae . In two complementary experiments, isotope-coded affinity tags and tandem mass spectrometry were used to quantify the relative enrichment of proteins during the purification of peroxisomes. Mathematical modeling of the data from 306 quantified proteins led to a prioritized list of 70 candidates whose enrichment scores indicated a high likelihood of them being peroxisomal. Among these proteins, eight novel peroxisome-associated proteins were identified. The top novel peroxisomal candidate was the small GTPase Rho1p. Although Rho1p has been shown to be tethered to membranes of the secretory pathway, we show that it is specifically recruited to peroxisomes upon their induction in a process dependent on its interaction with the peroxisome membrane protein Pex25p. Rho1p regulates the assembly state of actin on the peroxisome membrane, thereby controlling peroxisome membrane dynamics and biogenesis.
Access Privileges: [View/Edit]
SBEAMS 0.21-dev
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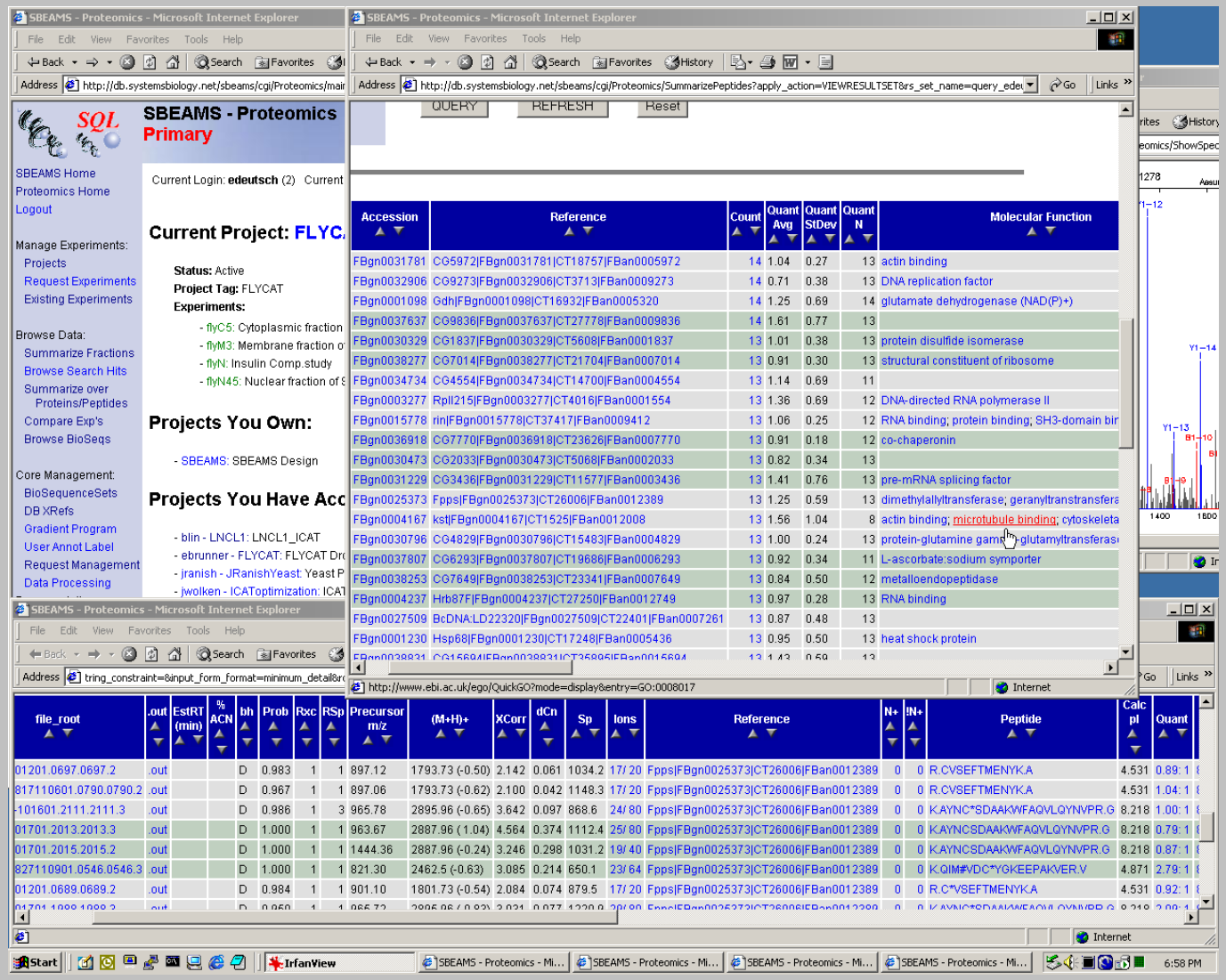
SBEAMS – Proteomics
Proteomics Analysis Database



SBEAMS – Proteomics: Goals

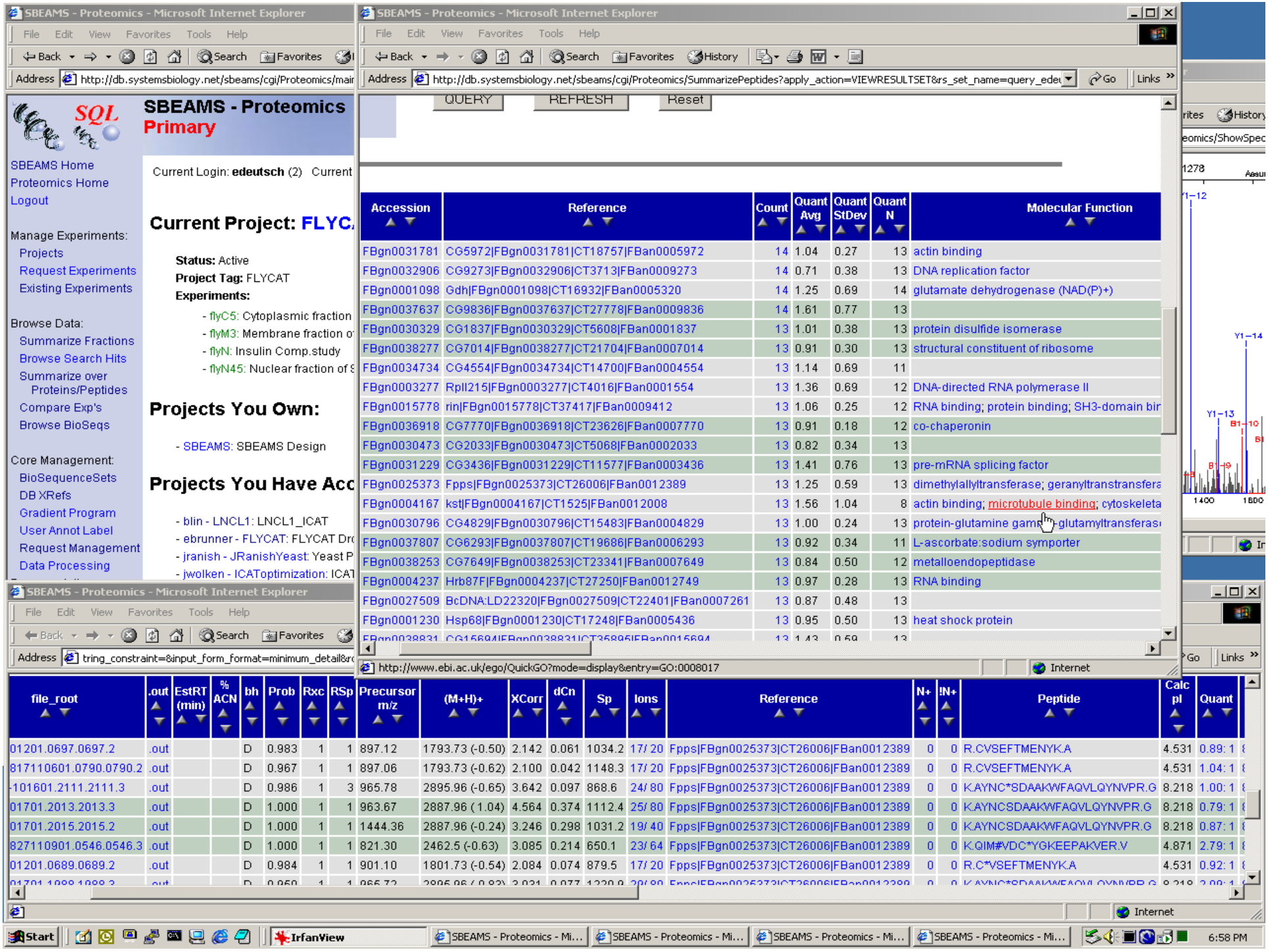
- Organize many projects/experiments/searches into relational database schema
- Tools to explore the search results similar to existing ways plus lots of new ways including comparison of multiple experiments
- Allow users to store annotations of search hits after personal validation
- Allow queries across multiple experiments to capitalize on previous annotations
- Designed for ISB high-throughput 2DLC mass-spec Proteomics experiments
- Manage data collection and analysis pipeline
- Annotated Peptide Database: library of observed peptides including their properties and conditions under which they were seen
- Provide a platform for further software development and analysis
- Integration with other modules/databases (e.g., Microarray)
- Data visualization with Cytoscape

SBEAMS – Proteomics: Main Features

- Project (Study) Information/Overview/Access Control
- Experimental information storage/access
- Comparison across experiments or search batches
- Quantitation summaries for one or more experiments
- Gene Ontology/InterPro annotation information
- Browse search_hit (ID'ed peptides) with spectra + Xpress

- Various metrics: Peptide probability scores, Xcorr, calc pI, Xpress values, etc.
- Calculation of % ACN with gradient program information

- Browse possible tryptic peptides for biosequence sets
- ProteinProphet output exploration
- Annotated Peptide Database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Primary
SBEAMS Home
Proteomics Home
Logout
Manage Experiments:
Projects
Request Experiments
Existing Experiments
Browse Data:
Summarize Fractions
Browse Search Hits
Summarize over Proteins/Peptides
Compare Exp's
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Core Management:
BioSequenceSets
DB XRefs
Gradient Program
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Request Management
Data Processing
Current Login: edeutsch (2) Current
Current Project: FLYC
Status: Active
Project Tag: FLYCAT
Experiments:
- flyC5: Cytoplasmic fraction
- flyM3: Membrane fraction o
- flyN: Insulin Comp.study
- flyN45: Nuclear fraction of
Projects You Own:
- SBEAMS: SBEAMS Design
Projects You Have Acc
- blin - LNCL1: LNCL1_ICAT
- ebrunner - FLYCAT: FLYCAT Dr
- jranish - JRanishYeast: Yeast P
- jwolken - ICAToptimization: ICAT
QUERY
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Molecular Function
FBgn0031781 CG5972|FBgn0031781|CT18757|FBan0005972 14 1.04 0.27 13 actin binding
FBgn0032906 CG9273|FBgn0032906|CT3713|FBan0009273 14 0.71 0.38 13 DNA replication factor
FBgn0001098 Gdh|FBgn0001098|CT16932|FBan0005320 14 1.25 0.69 14 glutamate dehydrogenase (NAD(P)+)
FBgn0037637 CG9836|FBgn0037637|CT27778|FBan0009836 14 1.61 0.77 13
FBgn0030329 CG1837|FBgn0030329|CT5608|FBan0001837 13 1.01 0.38 13 protein disulfide isomerase
FBgn0038277 CG7014|FBgn0038277|CT21704|FBan0007014 13 0.91 0.30 13 structural constituent of ribosome
FBgn0034734 CG4554|FBgn0034734|CT14700|FBan0004554 13 1.14 0.69 11
FBgn0003277 RpII215|FBgn0003277|CT4016|FBan0001554 13 1.36 0.69 12 DNA-directed RNA polymerase II
FBgn0015778 rin|FBgn0015778|CT37417|FBan0009412 13 1.06 0.25 12 RNA binding; protein binding; SH3-domain bir
FBgn0036918 CG7770|FBgn0036918|CT23626|FBan0007770 13 0.91 0.18 12 co-chaperonin
FBgn0030473 CG2033|FBgn0030473|CT5068|FBan0002033 13 0.82 0.34 13
FBgn0031229 CG3436|FBgn0031229|CT11577|FBan0003436 13 1.41 0.76 13 pre-mRNA splicing factor
FBgn0025373 Fpps|FBgn0025373|CT26006|FBan0012389 13 1.25 0.59 13 dimethylallyltransferase; geranyltranstransfera
FBgn0004167 kst|FBgn0004167|CT1525|FBan0012008 13 1.56 1.04 8 actin binding; microtubule binding; cytoskeleta
FBgn0030796 CG4829|FBgn0030796|CT15483|FBan0004829 13 1.00 0.24 13 protein-glutamine gam -glutamyltransferas
FBgn0037807 CG6293|FBgn0037807|CT19686|FBan0006293 13 0.92 0.34 11 L-ascorbate:sodium symporter
FBgn0038253 CG7649|FBgn0038253|CT23341|FBan0007649 13 0.84 0.50 12 metalloendopeptidase
FBgn0004237 Hrb87F|FBgn0004237|CT27250|FBan0012749 13 0.97 0.28 13 RNA binding
FBgn0027509 BcDNA:LD22320|FBgn0027509|CT22401|FBan0007261 13 0.87 0.48 13
FBgn0001230 Hsp68|FBgn0001230|CT17248|FBan0005436 13 0.95 0.50 13 heat shock protein
http://www.ebi.ac.uk/ego/QuickGO?mode=display&entry=GO:0008017
Internet
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Precursor m/z
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XCorr
dCn
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Peptide
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01201.0697.0697.2 .out D 0.983 1 1 897.12 1793.73 (-0.50) 2.142 0.061 1034.2 17/ 20 Fpps|FBgn0025373|CT26006|FBan0012389 0 0 R.CVSEFTMENYK.A 4.531 0.89: 1
817110601.0790.0790.2 .out D 0.967 1 1 897.06 1793.73 (-0.62) 2.100 0.042 1148.3 17/ 20 Fpps|FBgn0025373|CT26006|FBan0012389 0 0 R.CVSEFTMENYK.A 4.531 1.04: 1
-101601.2111.2111.3 .out D 0.986 1 3 965.78 2895.96 (-0.65) 3.642 0.097 868.6 24/ 80 Fpps|FBgn0025373|CT26006|FBan0012389 0 0 K.AYNC*SDAAKWFAQVLQYNVPR.G 8.218 1.00: 1
01701.2013.2013.3 .out D 1.000 1 1 963.67 2887.96 (1.04) 4.564 0.374 1112.4 25/ 80 Fpps|FBgn0025373|CT26006|FBan0012389 0 0 K.AYNCSDAAKWFAQVLQYNVPR.G 8.218 0.79: 1
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827110901.0546.0546.3 .out D 1.000 1 1 821.30 2462.5 (-0.63) 3.085 0.214 650.1 23/ 64 Fpps|FBgn0025373|CT26006|FBan0012389 0 0 K.QIM#VDC*YGKEEPAKVER.V 4.871 2.79: 1
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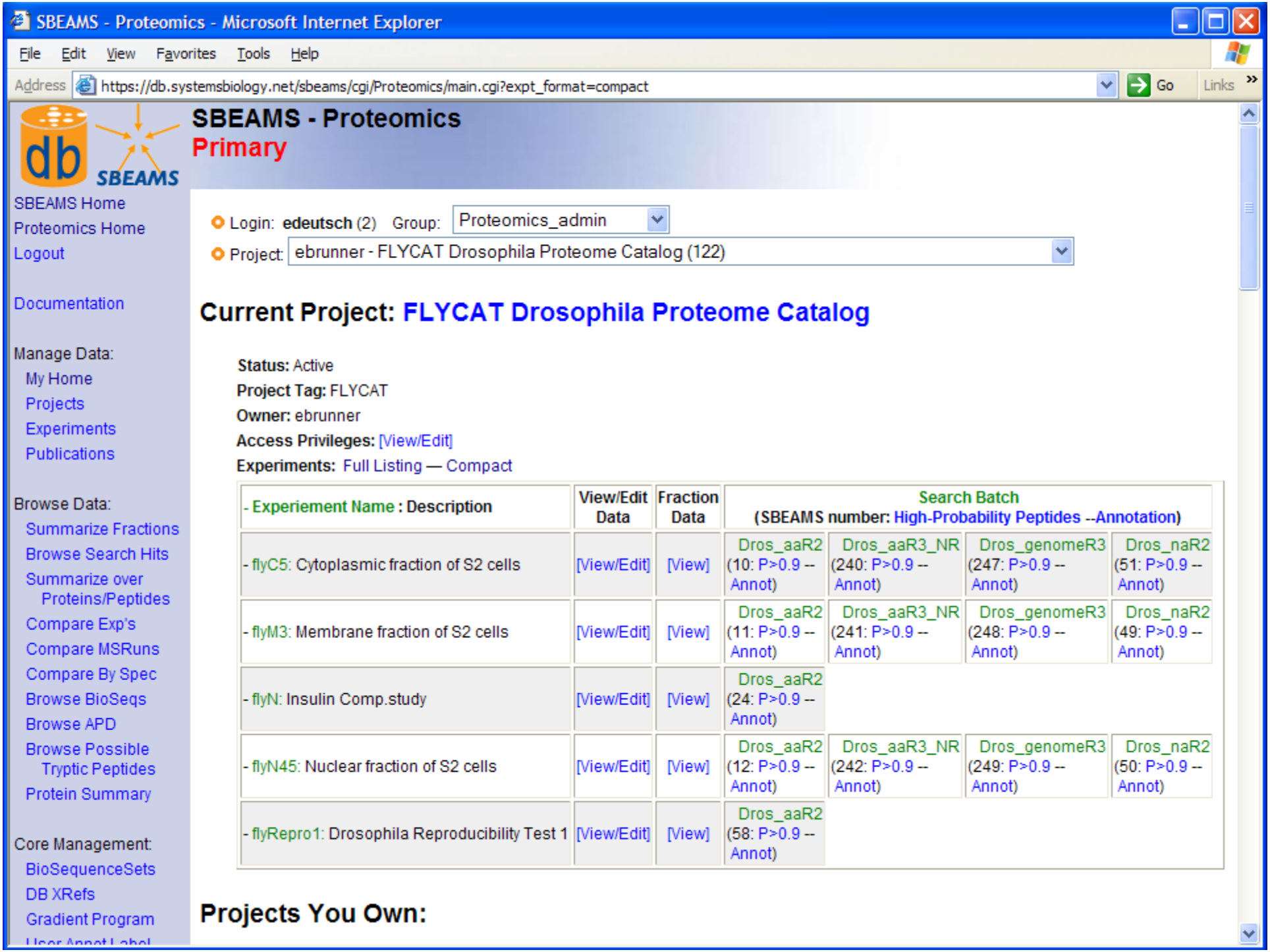
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Experiments
Publications
Browse Data:
Summarize Fractions
Browse Search Hits
Summarize over Proteins/Peptides
Compare Exp's
Compare MSRuns
Compare By Spec
Browse BioSeqs
Browse APD
Browse Possible Tryptic Peptides
Protein Summary
Core Management:
BioSequenceSets
DB XRefs
Gradient Program
Login: edeutsch (2) Group: Proteomics_admin
Project: ebrunner - FLYCAT Drosophila Proteome Catalog (122)
Current Project: FLYCAT Drosophila Proteome Catalog
Status: Active
Project Tag: FLYCAT
Owner: ebrunner
Access Privileges: [View/Edit]
Experiments: Full Listing — Compact
- Experiement Name : Description
View/Edit Data
Fraction Data
Search Batch (SBEAMS number: High-Probability Peptides --Annotation)
- flyC5: Cytoplasmic fraction of S2 cells
[View/Edit]
[View]
Dros_aaR2 (10: P>0.9 -- Annot)
Dros_aaR3_NR (240: P>0.9 -- Annot)
Dros_genomeR3 (247: P>0.9 -- Annot)
Dros_naR2 (51: P>0.9 -- Annot)
- flyM3: Membrane fraction of S2 cells
[View/Edit]
[View]
Dros_aaR2 (11: P>0.9 -- Annot)
Dros_aaR3_NR (241: P>0.9 -- Annot)
Dros_genomeR3 (248: P>0.9 -- Annot)
Dros_naR2 (49: P>0.9 -- Annot)
- flyN: Insulin Comp.study
[View/Edit]
[View]
Dros_aaR2 (24: P>0.9 -- Annot)
- flyN45: Nuclear fraction of S2 cells
[View/Edit]
[View]
Dros_aaR2 (12: P>0.9 -- Annot)
Dros_aaR3_NR (242: P>0.9 -- Annot)
Dros_genomeR3 (249: P>0.9 -- Annot)
Dros_naR2 (50: P>0.9 -- Annot)
- flyRepro1: Drosophila Reproducibility Test 1
[View/Edit]
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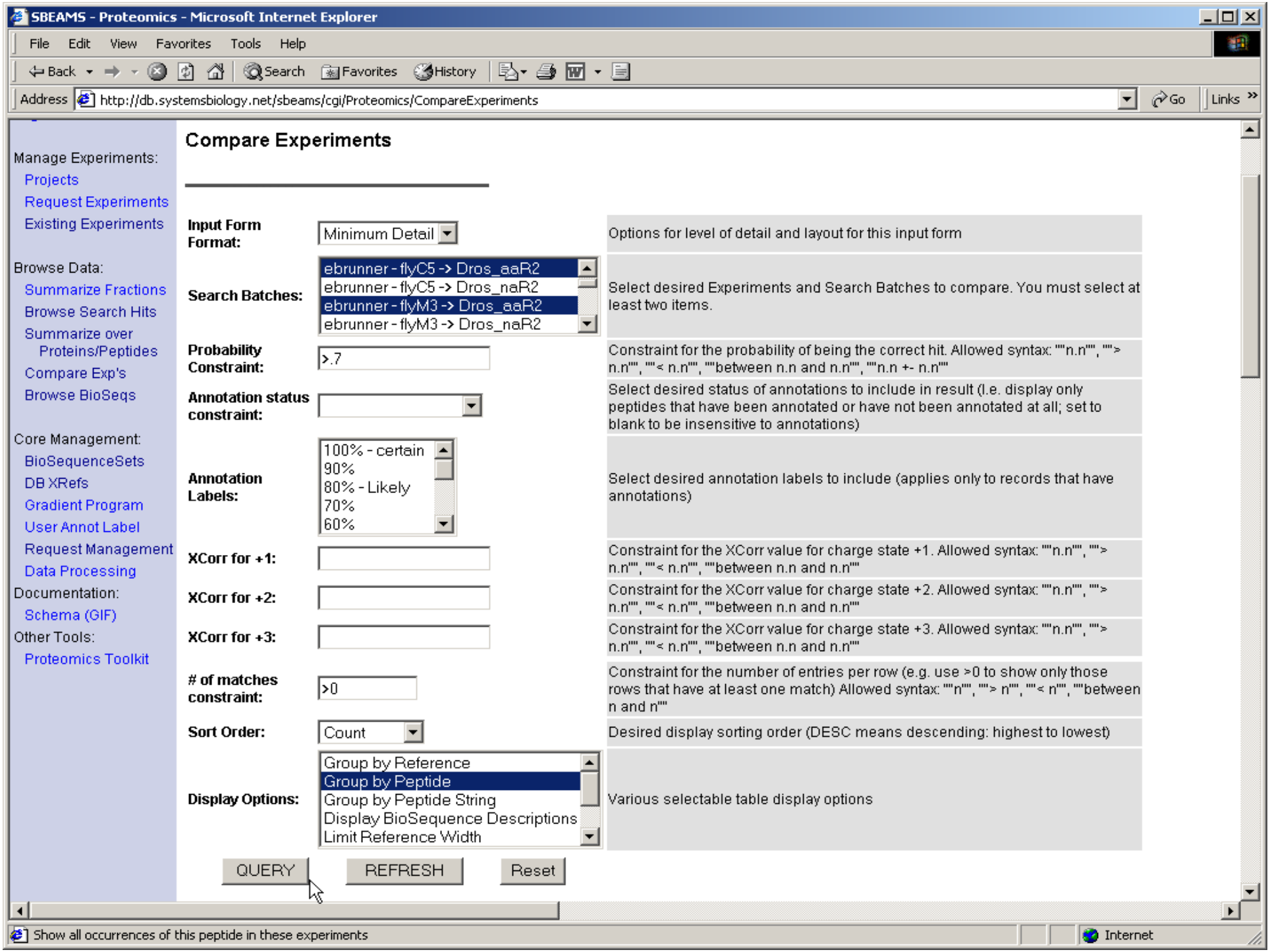
Dros_aaR2 (58: P>0.9 -- Annot)
Projects You Own: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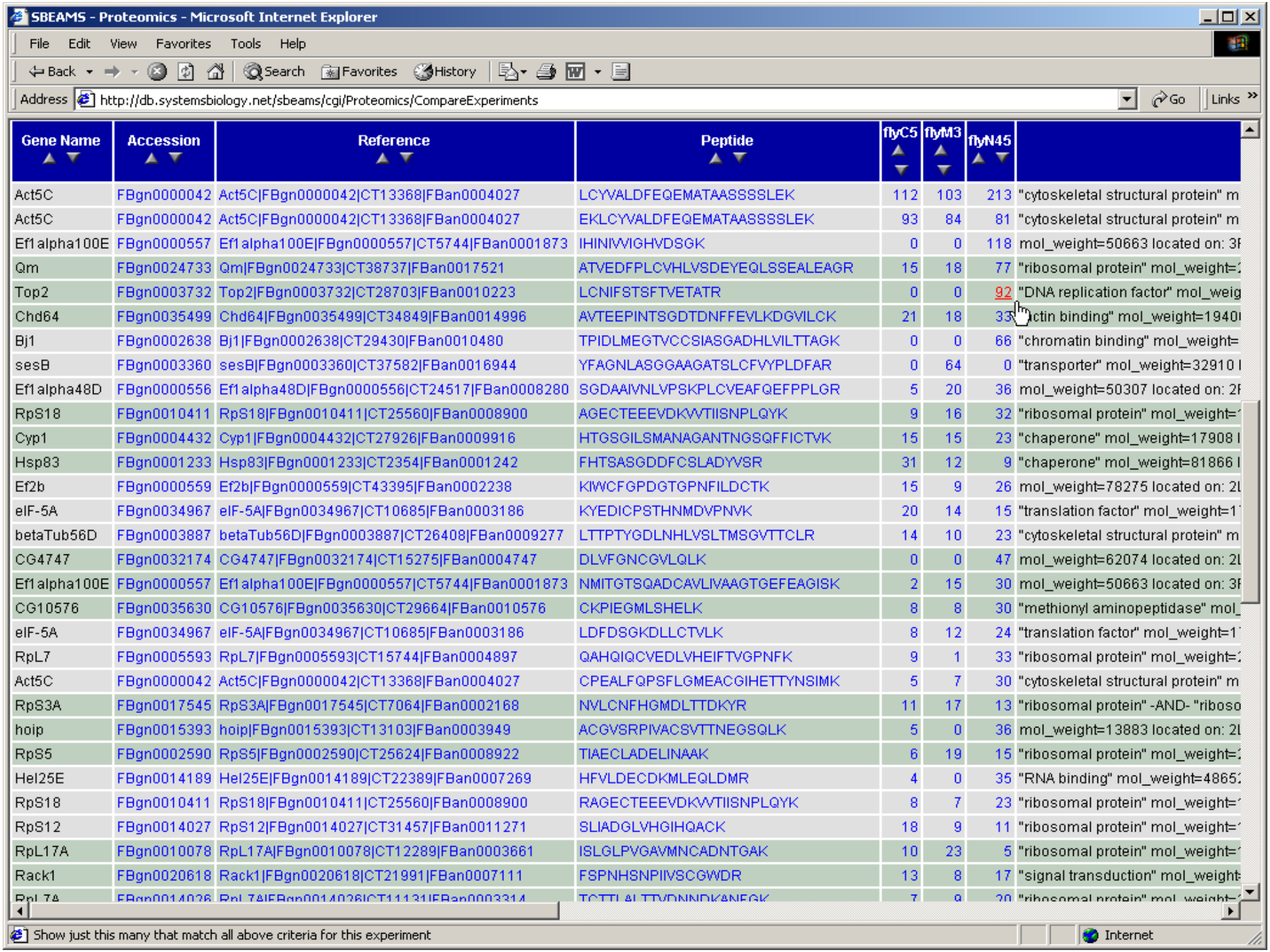
Address http://db.systemsbiology.net/sbeams/cgi/Proteomics/CompareExperiments
Go Links
Manage Experiments:
Projects
Request Experiments
Existing Experiments
Browse Data:
Summarize Fractions
Browse Search Hits
Summarize over Proteins/Peptides
Compare Exp's
Browse BioSeqs
Core Management:
BioSequenceSets
DB XRefs
Gradient Program
User Annot Label
Request Management
Data Processing
Documentation:
Schema (GIF)
Other Tools:
Proteomics Toolkit
Compare Experiments
Input Form Format:
Minimum Detail
Options for level of detail and layout for this input form
Search Batches:
ebrunner - flyC5 -> Dros_aaR2
ebrunner - flyC5 -> Dros_naR2
ebrunner - flyM3 -> Dros_aaR2
ebrunner - flyM3 -> Dros_naR2
Select desired Experiments and Search Batches to compare. You must select at least two items.
Probability Constraint:
>.7
Constraint for the probability of being the correct hit. Allowed syntax: ""n.n"", "">n.n"", ""< n.n"", ""between n.n and n.n"", ""n.n +- n.n""
Annotation status constraint:
Select desired status of annotations to include in result (i.e. display only peptides that have been annotated or have not been annotated at all; set to blank to be insensitive to annotations)
Annotation Labels:
100% - certain
90%
80% - Likely
70%
60%
Select desired annotation labels to include (applies only to records that have annotations)
XCorr for +1:
Constraint for the XCorr value for charge state +1. Allowed syntax: ""n.n"", "">n.n"", ""< n.n"", ""between n.n and n.n""
XCorr for +2:
Constraint for the XCorr value for charge state +2. Allowed syntax: ""n.n"", "">n.n"", ""< n.n"", ""between n.n and n.n""
XCorr for +3:
Constraint for the XCorr value for charge state +3. Allowed syntax: ""n.n"", "">n.n"", ""< n.n"", ""between n.n and n.n""
# of matches constraint:
>0
Constraint for the number of entries per row (e.g. use >0 to show only those rows that have at least one match) Allowed syntax: ""n"", "">n"", ""< n"", ""between n and n""
Sort Order:
Count
Desired display sorting order (DESC means descending: highest to lowest)
Display Options:
Group by Reference
Group by Peptide
Group by Peptide String
Display BioSequence Descriptions
Limit Reference Width
Various selectable table display options
QUERY
REFRESH
Reset
Show all occurrences of this peptide in these experiments
Internet



Gene Name	Accession	Reference	Peptide	flyC5	flyM3	flyN45	
Act5C	FBgn0000042	Act5C|FBgn0000042|CT13368|FBan0004027	LCYVALDFEQEMATAASSSSLEK	112	103	213	"cytoskeletal structural protein" m
Act5C	FBgn0000042	Act5C|FBgn0000042|CT13368|FBan0004027	EKLCYVALDFEQEMATAASSSSLEK	93	84	81	"cytoskeletal structural protein" m
Ef1alpha100E	FBgn0000557	Ef1alpha100E|FBgn0000557|CT5744|FBan0001873	IHINIVVIGHVDSGK	0	0	118	mol_weight=50663 located on: 3F
Qm	FBgn0024733	Qm|FBgn0024733|CT38737|FBan0017521	ATVEDFPLCVHLVSDEYEQLSSEALEAGR	15	18	77	"ribosomal protein" mol_weight=2
Top2	FBgn0003732	Top2|FBgn0003732|CT28703|FBan0010223	LCNIFSTSFTVETATR	0	0	92	"DNA replication factor" mol_weig
Chd64	FBgn0035499	Chd64|FBgn0035499|CT34849|FBan0014996	AVTEEPINTSGDTDNFFEVLKDGVILCK	21	18	33	ctin binding" mol_weight=1940
Bj1	FBgn0002638	Bj1|FBgn0002638|CT29430|FBan0010480	TPIDLMEGTVCCSIASGADHLVILTTAGK	0	0	66	"chromatin binding" mol_weight=
sesB	FBgn0003360	sesB|FBgn0003360|CT37582|FBan0016944	YFAGNLASGGAAGATSLCFVYPLDFAR	0	64	0	"transporter" mol_weight=32910 I
Ef1alpha48D	FBgn0000556	Ef1alpha48D|FBgn0000556|CT24517|FBan0008280	SGDAAIVNLVPSKPLCVEAFQEFPPLGR	5	20	36	mol_weight=50307 located on: 2F
RpS18	FBgn0010411	RpS18|FBgn0010411|CT25560|FBan0008900	AGECTEEEVDKVVTIISNPLQYK	9	16	32	"ribosomal protein" mol_weight=1
Cyp1	FBgn0004432	Cyp1|FBgn0004432|CT27926|FBan0009916	HTGSGILSMANAGANTNGSQFFICTVK	15	15	23	"chaperone" mol_weight=17908 I
Hsp83	FBgn0001233	Hsp83|FBgn0001233|CT2354|FBan0001242	FHTSASGDDFCSLADYVSR	31	12	9	"chaperone" mol_weight=81866 I
Ef2b	FBgn0000559	Ef2b|FBgn0000559|CT43395|FBan0002238	KIWCFGPDGTGPNFILDCTK	15	9	26	mol_weight=78275 located on: 2L
eIF-5A	FBgn0034967	eIF-5A|FBgn0034967|CT10685|FBan0003186	KYEDICPSTHNMDVPNVK	20	14	15	"translation factor" mol_weight=1
betaTub56D	FBgn0003887	betaTub56D|FBgn0003887|CT26408|FBan0009277	LTTPTYGDLNHLVSLTMSGVTTCLR	14	10	23	"cytoskeletal structural protein" m
CG4747	FBgn0032174	CG4747|FBgn0032174|CT15275|FBan0004747	DLVFGNCGVLQLK	0	0	47	mol_weight=62074 located on: 2L
Ef1alpha100E	FBgn0000557	Ef1alpha100E|FBgn0000557|CT5744|FBan0001873	NMITGTSQADCAVLIVAAGTGEFEAGISK	2	15	30	mol_weight=50663 located on: 3F
CG10576	FBgn0035630	CG10576|FBgn0035630|CT29664|FBan0010576	CKPIEGMLSHELK	8	8	30	"methionyl aminopeptidase" mol_
eIF-5A	FBgn0034967	eIF-5A|FBgn0034967|CT10685|FBan0003186	LDFDSGKDLLCTVLK	8	12	24	"translation factor" mol_weight=1
RpL7	FBgn0005593	RpL7|FBgn0005593|CT15744|FBan0004897	QAHQIQCVEDLVHEIFTVGPNFK	9	1	33	"ribosomal protein" mol_weight=2
Act5C	FBgn0000042	Act5C|FBgn0000042|CT13368|FBan0004027	CPEALFQPSFLGMEACGIHETTYNSIMK	5	7	30	"cytoskeletal structural protein" m
RpS3A	FBgn0017545	RpS3A|FBgn0017545|CT7064|FBan0002168	NVLCNFHGMDLTTDKYR	11	17	13	"ribosomal protein" -AND- "riboso
hoip	FBgn0015393	hoip|FBgn0015393|CT13103|FBan0003949	ACGVSRPIVACSVTTNEGSQLK	5	0	36	mol_weight=13883 located on: 2L
RpS5	FBgn0002590	RpS5|FBgn0002590|CT25624|FBan0008922	TIAECLADELINAAK	6	19	15	"ribosomal protein" mol_weight=2
Hel25E	FBgn0014189	Hel25E|FBgn0014189|CT22389|FBan0007269	HFVLDECDKMLEQLDMR	4	0	35	"RNA binding" mol_weight=4865
RpS18	FBgn0010411	RpS18|FBgn0010411|CT25560|FBan0008900	RAGECTEEEVDKVVTIISNPLQYK	8	7	23	"ribosomal protein" mol_weight=1
RpS12	FBgn0014027	RpS12|FBgn0014027|CT31457|FBan0011271	SLIADGLVHGIHQACK	18	9	11	"ribosomal protein" mol_weight=1
RpL17A	FBgn0010078	RpL17A|FBgn0010078|CT12289|FBan0003661	ISLGLPVGAVMNCADNTGAK	10	23	5	"ribosomal protein" mol_weight=1
Rack1	FBgn0020618	Rack1|FBgn0020618|CT21991|FBan0007111	FSPNHSNPIIVSCGWDR	13	8	17	"signal transduction" mol_weight=
RpL7A	FBgn0014026	RpL7A|FBgn0014026|CT11131|FBan0003314	TCTTLALTTVDNNDKANEGK	7	9	20	"ribosomal protein" mol_weight=1

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Ef2b	FBgn0000559	Ef2b|FBgn0000559|CT43395|FBan0002238	SCDPDGPLMMYISK	8	13	11	mol_weight=78275 located on: 2L 39E
alphaTub84B	FBgn0003884	alphaTub84B|FBgn0003884|CT42823|FBan0001913	AVCMLSNTTAIAEAWAR	25	3	3	mol_weight=47339 located on: 3R 84C
CG7176	FBgn0035881	CG7176|FBgn0035881|CT22163|FBan0007176	AKLDNNEPLKQFADTLEQVCIDTIESGAMTK	12	9	10	"enzyme" mol_weight=52590 located o
Ef2b	FBgn0000559	Ef2b|FBgn0000559|CT43395|FBan0002238	CLYAAAITAKPR	11	0	20	mol_weight=78275 located on: 2L 39E
RpL22	FBgn0015288	RpL22|FBgn0015288|CT22861|FBan0007434	FTIDCTNIAEDSIMDVADFEK	3	18	10	"ribosomal protein" mol_weight=30610
CG7176	FBgn0035881	CG7176|FBgn0035881|CT22163|FBan0007176	LDNNEPLKQFADTLEQVCIDTIESGAMTK	6	15	9	"enzyme" mol_weight=52590 located o

Displayed rows 1 - 50 of 4301

Result Page

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51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 of 87

Page Size: 50 Page Number: 1 VIEWRESULTSET

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URL to re-execute this query: http://db.systemsbiology.net/dev2/sbeams/cgi/Proteomics/CompareExperiments?apply_action=QUERY&input_form_format=minimum_detail&row_limit=5000&pi

Summary of resultset:

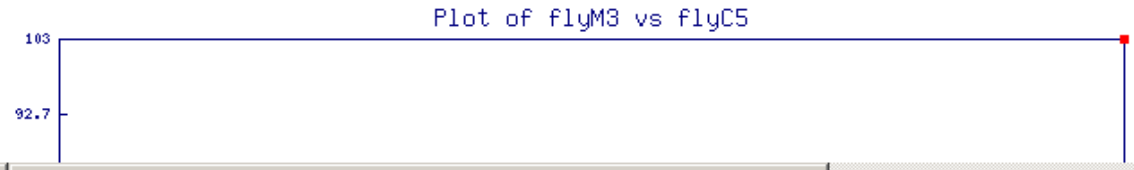
Total number of Peptides: 4301

Number of Peptides seen in every experiment: 419

Number of Peptides seen more than once in every experiment: 230

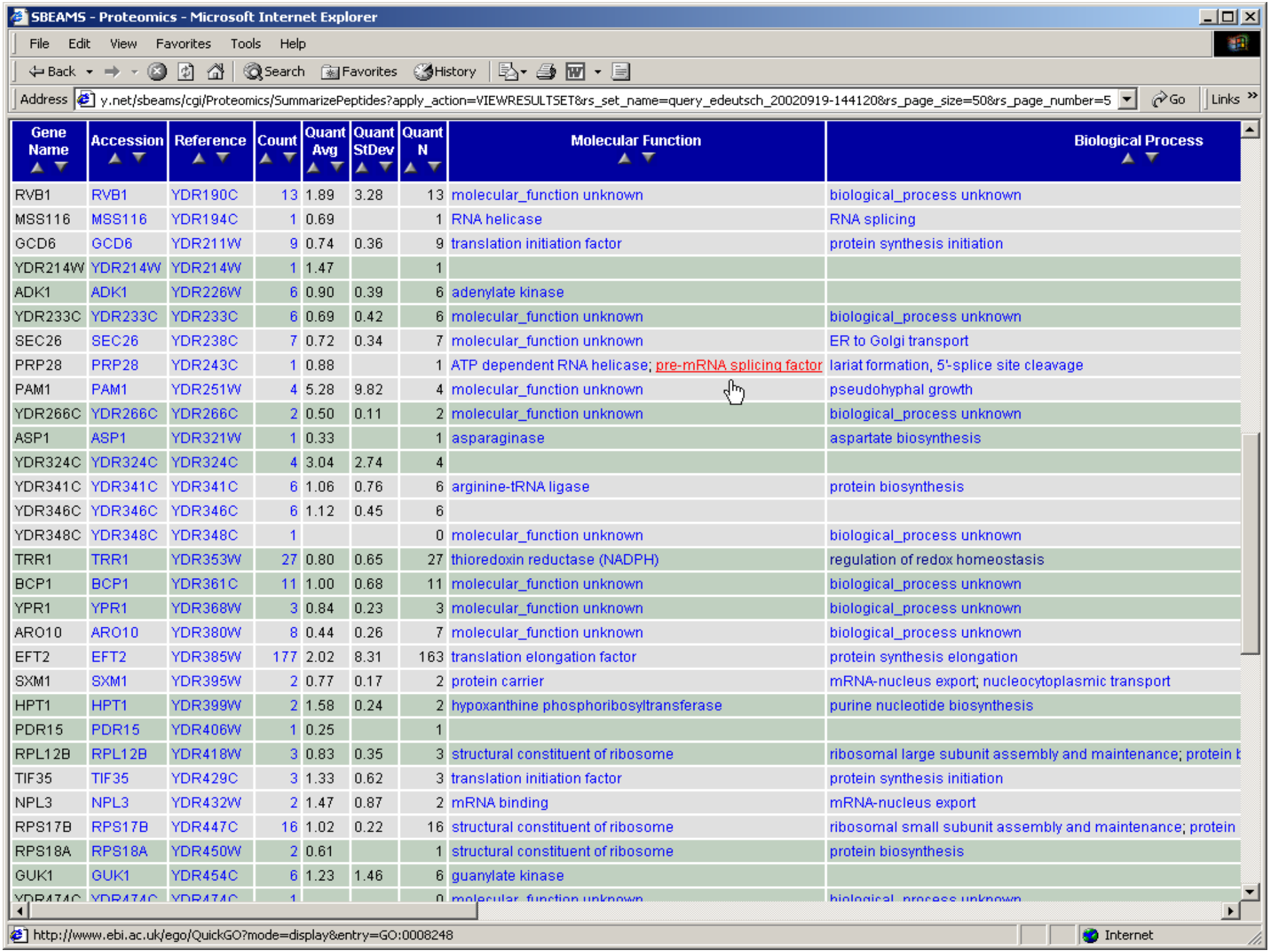
Intersection of observed Peptides in experiments:

-	flyC5	flyM3	flyN45
flyC5	1413	555	712
flyM3		1903	707
flyN45			2540

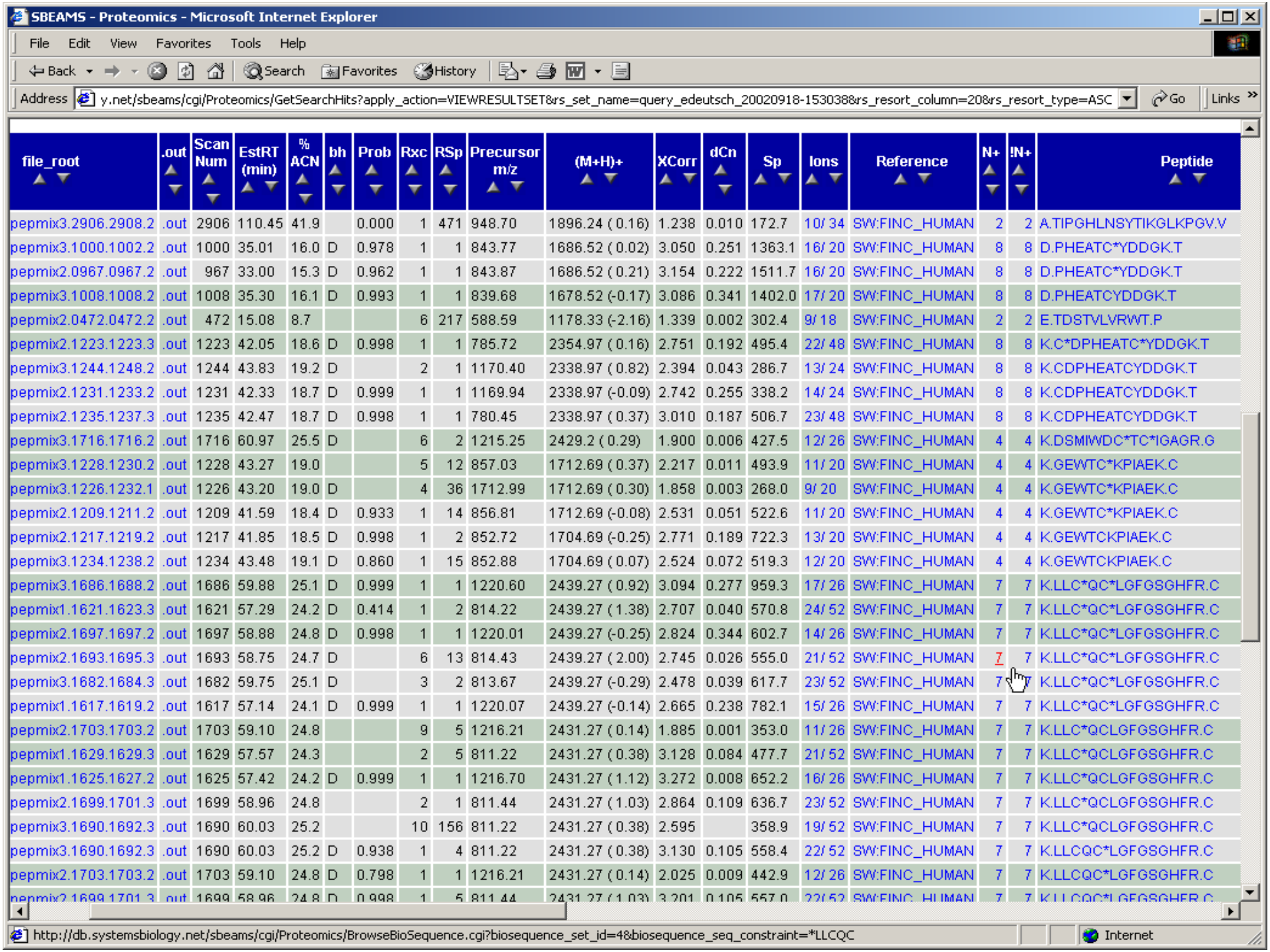


Show all occurrences of this peptide in these experiments

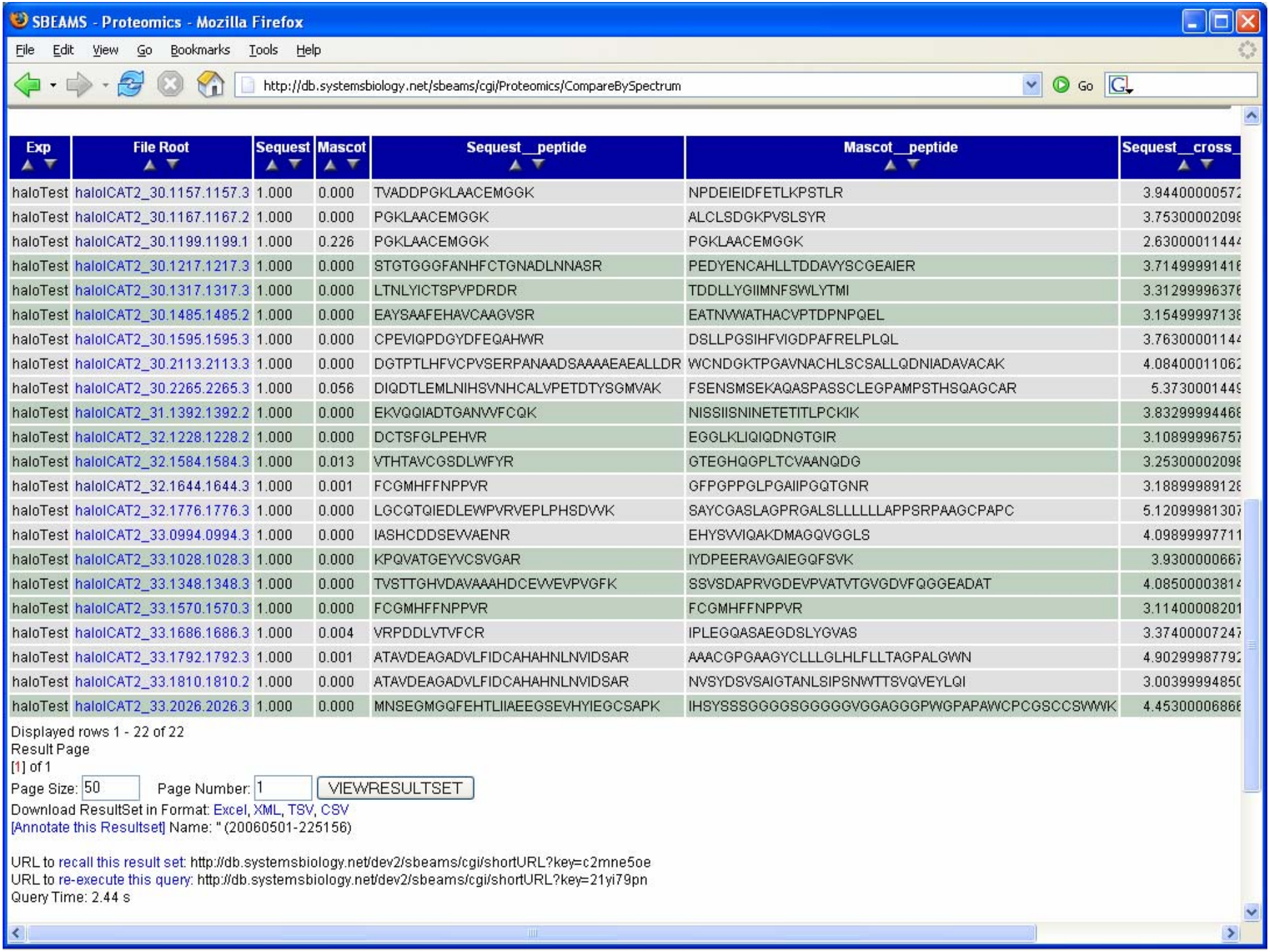
Internet



Gene Name	Accession	Reference	Count	Quant Avg	Quant StDev	Quant N	Molecular Function	Biological Process
RVB1	RVB1	YDR190C	13	1.89	3.28	13	molecular_function unknown	biological_process unknown
MSS116	MSS116	YDR194C	1	0.69		1	RNA helicase	RNA splicing
GCD6	GCD6	YDR211W	9	0.74	0.36	9	translation initiation factor	protein synthesis initiation
YDR214W	YDR214W	YDR214W	1	1.47		1		
ADK1	ADK1	YDR226W	6	0.90	0.39	6	adenylate kinase	
YDR233C	YDR233C	YDR233C	6	0.69	0.42	6	molecular_function unknown	biological_process unknown
SEC26	SEC26	YDR238C	7	0.72	0.34	7	molecular_function unknown	ER to Golgi transport
PRP28	PRP28	YDR243C	1	0.88		1	ATP dependent RNA helicase; pre-mRNA splicing factor	lariat formation, 5'-splice site cleavage
PAM1	PAM1	YDR251W	4	5.28	9.82	4	molecular_function unknown	pseudohyphal growth
YDR266C	YDR266C	YDR266C	2	0.50	0.11	2	molecular_function unknown	biological_process unknown
ASP1	ASP1	YDR321W	1	0.33		1	asparaginase	aspartate biosynthesis
YDR324C	YDR324C	YDR324C	4	3.04	2.74	4		
YDR341C	YDR341C	YDR341C	6	1.06	0.76	6	arginine-tRNA ligase	protein biosynthesis
YDR346C	YDR346C	YDR346C	6	1.12	0.45	6		
YDR348C	YDR348C	YDR348C	1			0	molecular_function unknown	biological_process unknown
TRR1	TRR1	YDR353W	27	0.80	0.65	27	thioredoxin reductase (NADPH)	regulation of redox homeostasis
BCP1	BCP1	YDR361C	11	1.00	0.68	11	molecular_function unknown	biological_process unknown
YPR1	YPR1	YDR368W	3	0.84	0.23	3	molecular_function unknown	biological_process unknown
ARO10	ARO10	YDR380W	8	0.44	0.26	7	molecular_function unknown	biological_process unknown
EFT2	EFT2	YDR385W	177	2.02	8.31	163	translation elongation factor	protein synthesis elongation
SXM1	SXM1	YDR395W	2	0.77	0.17	2	protein carrier	mRNA-nucleus export; nucleocytoplasmic transport
HPT1	HPT1	YDR399W	2	1.58	0.24	2	hypoxanthine phosphoribosyltransferase	purine nucleotide biosynthesis
PDR15	PDR15	YDR406W	1	0.25		1		
RPL12B	RPL12B	YDR418W	3	0.83	0.35	3	structural constituent of ribosome	ribosomal large subunit assembly and maintenance; protein t
TIF35	TIF35	YDR429C	3	1.33	0.62	3	translation initiation factor	protein synthesis initiation
NPL3	NPL3	YDR432W	2	1.47	0.87	2	mRNA binding	mRNA-nucleus export
RPS17B	RPS17B	YDR447C	16	1.02	0.22	16	structural constituent of ribosome	ribosomal small subunit assembly and maintenance; protein
RPS18A	RPS18A	YDR450W	2	0.61		1	structural constituent of ribosome	protein biosynthesis
GUK1	GUK1	YDR454C	6	1.23	1.46	6	guanylate kinase	
YDR474C	YDR474C	YDR474C	1			0	molecular_function unknown	biological_process unknown



file_root	.out	Scan Num	EstRT (min)	% ACN	bh	Prob	Rxc	RSp	Precursor m/z	(M+H)+	XCorr	dCn	Sp	Ions	Reference	N+	!N+	Peptide
pepmix3.2906.2908.2	.out	2906	110.45	41.9		0.000	1	471	948.70	1896.24 (0.16)	1.238	0.010	172.7	10/ 34	SW:FINC_HUMAN	2	2	A.TIPGHLNSYTIKGLKPGV.V
pepmix3.1000.1002.2	.out	1000	35.01	16.0	D	0.978	1	1	843.77	1686.52 (0.02)	3.050	0.251	1363.1	16/ 20	SW:FINC_HUMAN	8	8	D.PHEATC*YDDGK.T
pepmix2.0967.0967.2	.out	967	33.00	15.3	D	0.962	1	1	843.87	1686.52 (0.21)	3.154	0.222	1511.7	16/ 20	SW:FINC_HUMAN	8	8	D.PHEATC*YDDGK.T
pepmix3.1008.1008.2	.out	1008	35.30	16.1	D	0.993	1	1	839.68	1678.52 (-0.17)	3.086	0.341	1402.0	17/ 20	SW:FINC_HUMAN	8	8	D.PHEATCYDDGK.T
pepmix2.0472.0472.2	.out	472	15.08	8.7			6	217	588.59	1178.33 (-2.16)	1.339	0.002	302.4	9/ 18	SW:FINC_HUMAN	2	2	E.TDSTVLVRWT.P
pepmix2.1223.1223.3	.out	1223	42.05	18.6	D	0.998	1	1	785.72	2354.97 (0.16)	2.751	0.192	495.4	22/ 48	SW:FINC_HUMAN	8	8	K.C*DPHEATC*YDDGK.T
pepmix3.1244.1248.2	.out	1244	43.83	19.2	D		2	1	1170.40	2338.97 (0.82)	2.394	0.043	286.7	13/ 24	SW:FINC_HUMAN	8	8	K.CDPHEATCYDDGK.T
pepmix2.1231.1233.2	.out	1231	42.33	18.7	D	0.999	1	1	1169.94	2338.97 (-0.09)	2.742	0.255	338.2	14/ 24	SW:FINC_HUMAN	8	8	K.CDPHEATCYDDGK.T
pepmix2.1235.1237.3	.out	1235	42.47	18.7	D	0.998	1	1	780.45	2338.97 (0.37)	3.010	0.187	506.7	23/ 48	SW:FINC_HUMAN	8	8	K.CDPHEATCYDDGK.T
pepmix3.1716.1716.2	.out	1716	60.97	25.5	D		6	2	1215.25	2429.2 (0.29)	1.900	0.006	427.5	12/ 26	SW:FINC_HUMAN	4	4	K.DSMWDC*TC*IGAGR.G
pepmix3.1228.1230.2	.out	1228	43.27	19.0			5	12	857.03	1712.69 (0.37)	2.217	0.011	493.9	11/ 20	SW:FINC_HUMAN	4	4	K.GEWTC*KPIAEK.C
pepmix3.1226.1232.1	.out	1226	43.20	19.0	D		4	36	1712.99	1712.69 (0.30)	1.858	0.003	268.0	9/ 20	SW:FINC_HUMAN	4	4	K.GEWTC*KPIAEK.C
pepmix2.1209.1211.2	.out	1209	41.59	18.4	D	0.933	1	14	856.81	1712.69 (-0.08)	2.531	0.051	522.6	11/ 20	SW:FINC_HUMAN	4	4	K.GEWTC*KPIAEK.C
pepmix2.1217.1219.2	.out	1217	41.85	18.5	D	0.998	1	2	852.72	1704.69 (-0.25)	2.771	0.189	722.3	13/ 20	SW:FINC_HUMAN	4	4	K.GEWTCKPIAEK.C
pepmix3.1234.1238.2	.out	1234	43.48	19.1	D	0.860	1	15	852.88	1704.69 (0.07)	2.524	0.072	519.3	12/ 20	SW:FINC_HUMAN	4	4	K.GEWTCKPIAEK.C
pepmix3.1686.1688.2	.out	1686	59.88	25.1	D	0.999	1	1	1220.60	2439.27 (0.92)	3.094	0.277	959.3	17/ 26	SW:FINC_HUMAN	7	7	K.LLC*QC*LGFGSGHFR.C
pepmix1.1621.1623.3	.out	1621	57.29	24.2	D	0.414	1	2	814.22	2439.27 (1.38)	2.707	0.040	570.8	24/ 52	SW:FINC_HUMAN	7	7	K.LLC*QC*LGFGSGHFR.C
pepmix2.1697.1697.2	.out	1697	58.88	24.8	D	0.998	1	1	1220.01	2439.27 (-0.25)	2.824	0.344	602.7	14/ 26	SW:FINC_HUMAN	7	7	K.LLC*QC*LGFGSGHFR.C
pepmix2.1693.1695.3	.out	1693	58.75	24.7	D		6	13	814.43	2439.27 (2.00)	2.745	0.026	555.0	21/ 52	SW:FINC_HUMAN	7	7	K.LLC*QC*LGFGSGHFR.C
pepmix3.1682.1684.3	.out	1682	59.75	25.1	D		3	2	813.67	2439.27 (-0.29)	2.478	0.039	617.7	23/ 52	SW:FINC_HUMAN	7	7	K.LLC*QC*LGFGSGHFR.C
pepmix1.1617.1619.2	.out	1617	57.14	24.1	D	0.999	1	1	1220.07	2439.27 (-0.14)	2.665	0.238	782.1	15/ 26	SW:FINC_HUMAN	7	7	K.LLC*QC*LGFGSGHFR.C
pepmix2.1703.1703.2	.out	1703	59.10	24.8			9	5	1216.21	2431.27 (0.14)	1.885	0.001	353.0	11/ 26	SW:FINC_HUMAN	7	7	K.LLC*QCLGFGSGHFR.C
pepmix1.1629.1629.3	.out	1629	57.57	24.3			2	5	811.22	2431.27 (0.38)	3.128	0.084	477.7	21/ 52	SW:FINC_HUMAN	7	7	K.LLC*QCLGFGSGHFR.C
pepmix1.1625.1627.2	.out	1625	57.42	24.2	D	0.999	1	1	1216.70	2431.27 (1.12)	3.272	0.008	652.2	16/ 26	SW:FINC_HUMAN	7	7	K.LLC*QCLGFGSGHFR.C
pepmix2.1699.1701.3	.out	1699	58.96	24.8			2	1	811.44	2431.27 (1.03)	2.864	0.109	636.7	23/ 52	SW:FINC_HUMAN	7	7	K.LLC*QCLGFGSGHFR.C
pepmix3.1690.1692.3	.out	1690	60.03	25.2			10	156	811.22	2431.27 (0.38)	2.595		358.9	19/ 52	SW:FINC_HUMAN	7	7	K.LLC*QCLGFGSGHFR.C
pepmix3.1690.1692.3	.out	1690	60.03	25.2	D	0.938	1	4	811.22	2431.27 (0.38)	3.130	0.105	558.4	22/ 52	SW:FINC_HUMAN	7	7	K.LLCQC*LGFGSGHFR.C
pepmix2.1703.1703.2	.out	1703	59.10	24.8	D	0.798	1	1	1216.21	2431.27 (0.14)	2.025	0.009	442.9	12/ 26	SW:FINC_HUMAN	7	7	K.LLCQC*LGFGSGHFR.C
pepmix2.1699.1701.3	.out	1699	58.96	24.8	D	0.998	1	5	811.44	2431.27 (1.03)	3.201	0.105	557.0	22/ 52	SW:FINC_HUMAN	7	7	K.LLCQC*LGFGSGHFR.C



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haloTest	haloICAT2_30.1199.1199.1	1.000	0.226	PGKLAACEMGGK	PGKLAACEMGGK	2.63000011444
haloTest	haloICAT2_30.1217.1217.3	1.000	0.000	STGTGGGFANHFCTGNADLNNASR	PEDYENCAHLLTDDAVYSCGEAIER	3.71499991418
haloTest	haloICAT2_30.1317.1317.3	1.000	0.000	LTNLYICTSPVPDRDR	TDDLLYGIIMNFSWLYTMI	3.31299996378
haloTest	haloICAT2_30.1485.1485.2	1.000	0.000	EAYSAAFEHAVCAAGVSR	EATNVWATHACVPTDPNPQEL	3.15499997138
haloTest	haloICAT2_30.1595.1595.3	1.000	0.000	CPEVIQPDGYDFEQAHWR	DSLLPGSIHFVIGDPAFRELPLQL	3.76300001144
haloTest	haloICAT2_30.2113.2113.3	1.000	0.000	DGTPTLHFVCPVSERPANAADSAAAAEAEALLDR	WCNDGKTPGAVNACHLSCSALLQDNIADAVACAK	4.08400011062
haloTest	haloICAT2_30.2265.2265.3	1.000	0.056	DIQDTLEMLNIHSVNHCALVPETDTYSGMVAK	FSENSMSEKAQASPASSCLEGPAMPSTHSQAGCAR	5.37300014499
haloTest	haloICAT2_31.1392.1392.2	1.000	0.000	EKVQQIADTGANVVFCQK	NISSIISNINETETITLPCKIK	3.83299994468
haloTest	haloICAT2_32.1228.1228.2	1.000	0.000	DCTSFGLPEHVR	EGGLKLIQIQDNGTGIR	3.10899996757
haloTest	haloICAT2_32.1584.1584.3	1.000	0.013	VTHTAVCGSDLWFYR	GTEGHQGPLTCVAANQDG	3.25300002098
haloTest	haloICAT2_32.1644.1644.3	1.000	0.001	FCGMHFFNPPVR	GFPGPPGLPGAIIPGQTGNR	3.18899989128
haloTest	haloICAT2_32.1776.1776.3	1.000	0.000	LGCQTQIEDLEWPVRVEPLPHSDVVK	SAYCGASLAGPRGALSLLLLLLAPPSRPAAGCPAPC	5.12099981307
haloTest	haloICAT2_33.0994.0994.3	1.000	0.000	IASHCDDSEVVAENR	EHYSVVIQAKDMAGQVGGLS	4.09899997711
haloTest	haloICAT2_33.1028.1028.3	1.000	0.000	KPQVATGEYVCSVGAR	IYDPEERAVGAIEGQFSVK	3.93000000667
haloTest	haloICAT2_33.1348.1348.3	1.000	0.000	TVSTTGHVDAVAAAHDCEVVEVPVGFK	SSVSDAPRVGDEVPVATVTGVGDVFQGGEADAT	4.08500003814
haloTest	haloICAT2_33.1570.1570.3	1.000	0.000	FCGMHFFNPPVR	FCGMHFFNPPVR	3.11400008201
haloTest	haloICAT2_33.1686.1686.3	1.000	0.004	VRPDDLVTVFCR	IPLEGQASAEGDSLYGVAS	3.37400007247
haloTest	haloICAT2_33.1792.1792.3	1.000	0.001	ATAVDEAGADVLFIDCAHAHNLNVIDSAR	AAACGPGAAGYCLLLGLHLFLLTAGPALGWN	4.90299987792
haloTest	haloICAT2_33.1810.1810.2	1.000	0.000	ATAVDEAGADVLFIDCAHAHNLNVIDSAR	NVSYDSVSAIGTANLSIPSNWTTSVQVEYLQI	3.00399994850
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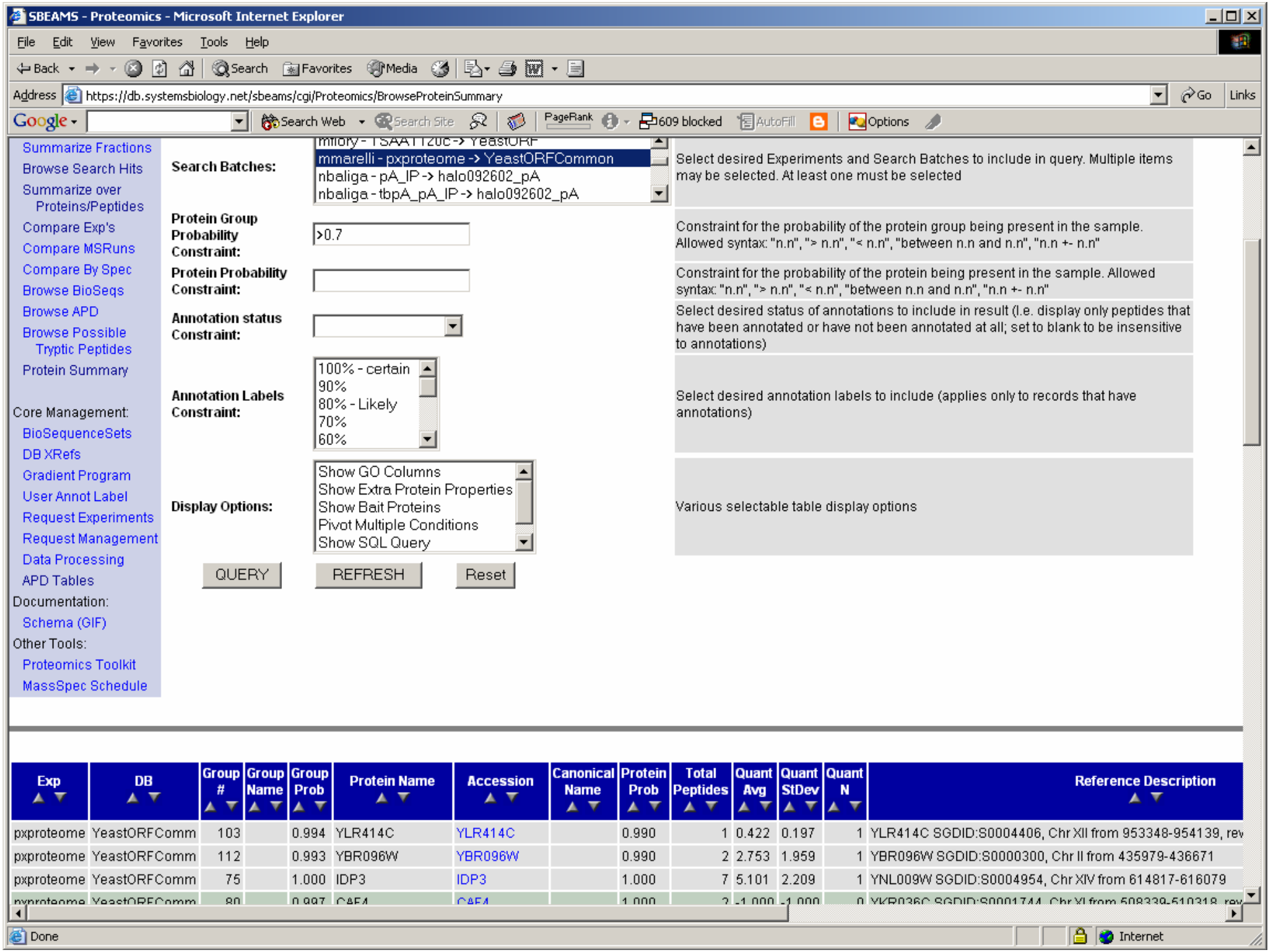

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pxproteome	YeastORFComm	112		0.993	YBR096W	YBR096W		0.990	2	2.753	1.959	1	YBR096W SGDID:S0000300, Chr II from 435979-436671
pxproteome	YeastORFComm	75		1.000	IDP3	IDP3		1.000	7	5.101	2.209	1	YNL009W SGDID:S0004954, Chr XIV from 614817-616079
pxproteome	YeastORFComm	80		0.997	CAF4	CAF4		1.000	2	-1.000	-1.000	0	YKR036C SGDID:S0001744, Chr XI from 508339-510318, rev

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Google Search Web Search Site PageRank 609 blocked AutoFill Options

pxproteome	YeastORFComm	31		1.000	SDH2	SDH2		1.000	4	1.938	0.004	2	YLL041C SGDID:S0003964, Chr XII from 53130-53930, revers
pxproteome	YeastORFComm	32		1.000	YIL108W	YIL108W		1.000	3	1.357	0.952	1	YIL108W SGDID:S0001370, Chr IX from 160884-162974
pxproteome	YeastORFComm	101		0.994	DOT6	DOT6		0.990	2				YER088C SGDID:S0000890, Chr V from 333172-335184, reve
pxproteome	YeastORFComm	100		0.994	EMP24	EMP24		0.990	1	2.662	0.363	1	YGL200C SGDID:S0003168, Chr VII from 122697-123308, rev
pxproteome	YeastORFComm	35		1.000	QCR6	QCR6		1.000	5	5.246	1.280	1	YFR033C SGDID:S0001929, Chr VI from 224313-224756, rev
pxproteome	YeastORFComm	102		0.994	RVB2	RVB2		0.990	2	-1.000	-1.000	1	YPL235W SGDID:S0006156, Chr XVI from 103232-104647
pxproteome	YeastORFComm	104		0.994	MSP1	MSP1		0.990	1	2.198	0.790	1	YGR028W SGDID:S0003260, Chr VII from 542197-543285
pxproteome	YeastORFComm	28		1.000	PEX6	PEX6	PEX6	1.000	7	4.349	1.695	3	YNL329C SGDID:S0005273, Chr XIV from 19541-22633, rever

Displayed rows 1 - 50 of 202
Result Page
[1] 2 3 4 5 of 5

Page Size: 50 Page Number: 1 VIEWRESULTSET

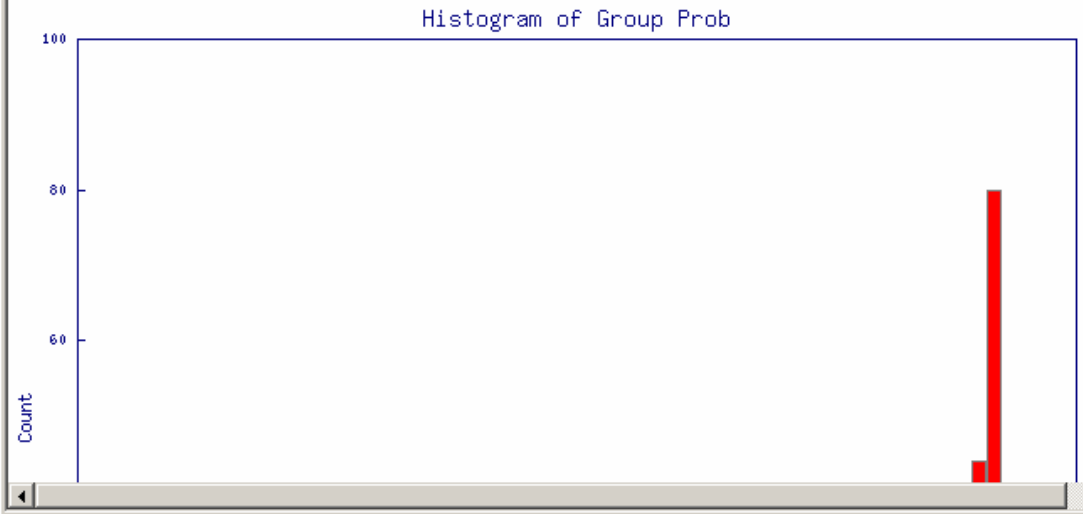
Download ResultSet in Format: Excel, XML, TSV, CSV

[View this Resultset with Cytoscape]

[Annotate this Resultset] Name: '' (2004-01-15 00:04:27)

URL to recall this result set: https://db.systemsbiology.net/sbeams/cgi/Proteomics/BrowseProteinSummary?apply_action=VIEWRESULTSET&rs_set_name=query_edeutsch_20040115-000346&rs_page_

URL to re-execute this query: https://db.systemsbiology.net/sbeams/cgi/Proteomics/BrowseProteinSummary?row_limit=50000&protein_group_probability_constraint=%3E0.7&input_form_format=minimur



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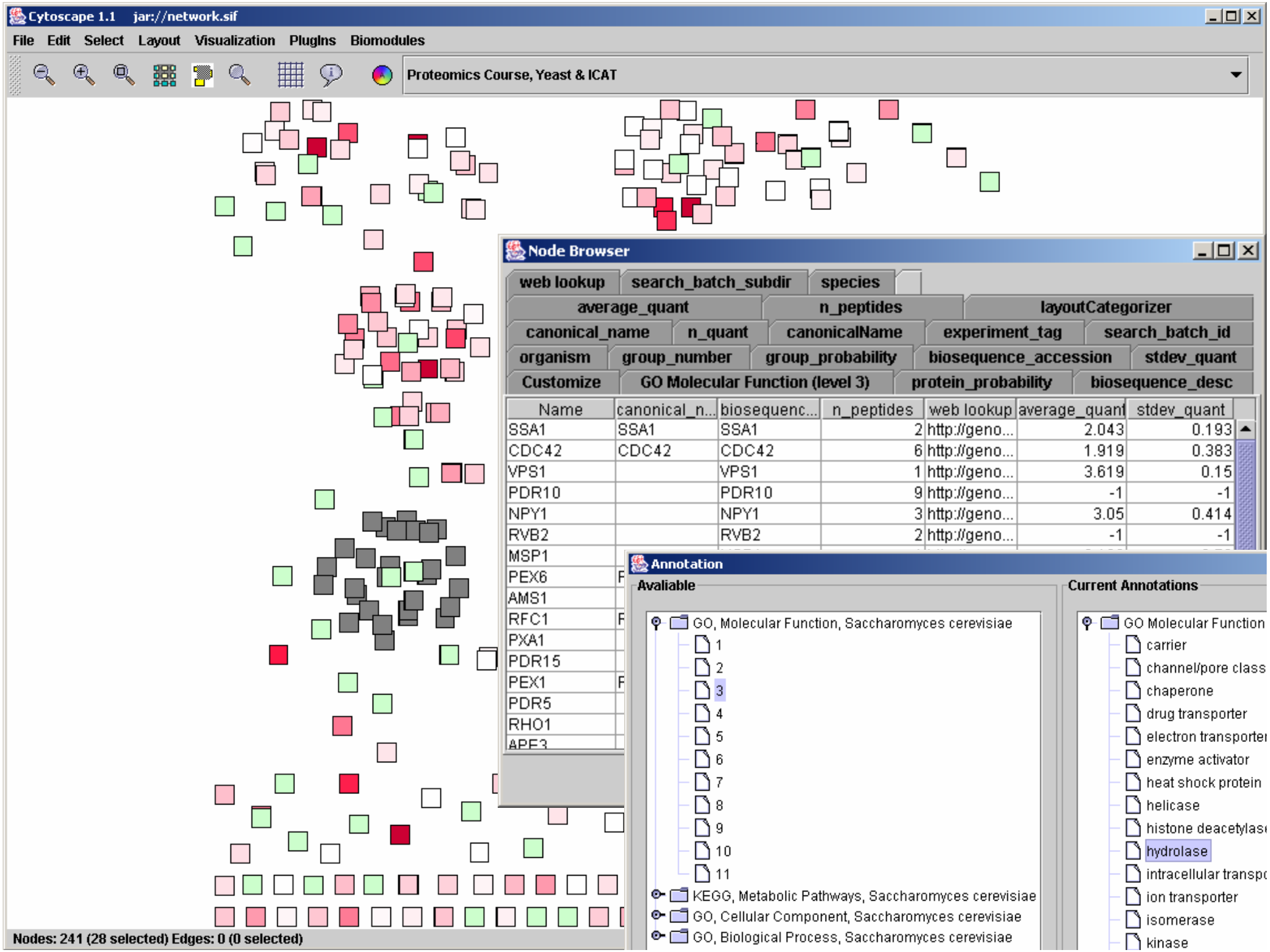
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experiment_tag
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organism
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biosequence_accession
stdev_quant
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CDC42 CDC42 CDC42 6 http://geno... 1.919 0.383
VPS1 VPS1 1 http://geno... 3.619 0.15
PDR10 PDR10 9 http://geno... -1 -1
NPY1 NPY1 3 http://geno... 3.05 0.414
RVB2 RVB2 2 http://geno... -1 -1
MSP1
PEX6
AMS1
RFC1
PXA1
PDR15
PEX1
PDR5
RHO1
Annotation
Avaliable
GO, Molecular Function, Saccharomyces cerevisiae
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3
4
5
6
7
8
9
10
11
KEGG, Metabolic Pathways, Saccharomyces cerevisiae
GO, Cellular Component, Saccharomyces cerevisiae
GO, Biological Process, Saccharomyces cerevisiae
Current Annotations
GO Molecular Function
carrier
channel/pore class
chaperone
drug transporter
electron transporter
enzyme activator
heat shock protein
helicase
histone deacetylase
hydrolase
intracellular transp
ion transporter
isomerase
kinase
Nodes: 241 (28 selected) Edges: 0 (0 selected)

SBEAMS – Proteomics

PRO

- Central repository of organized data
- Annotate results and capitalize on annotations of others
- Queries to compare/combine experiments
- Queries to search for the needle in the haystack
- Write your own queries if you know/learn SQL
- Cytoscape integration

CON

- Not a robust, streamlined system
- Needs lots of work
- No full-time support
- In some ways, harder to "do your own thing"
- Beware the resultset that is different from what you thought you asked for

SBEAMS – Proteomics
Data Exports and Data Standards

- Resultsets can be exported to Excel, XML, CSV, TSV
- Parts of the data model can be exported into XML format that follows the SBEAMS – Proteomics schema but not a standard

- MIAME for Microarrays (Minimum Information About a Microarray Experiment) (Brazma et al. 2001)
- MAGE-OM/ML for Microarrays (MicroArray Gene Expression Object Model/Markup Language) (Spellman et al. 2002)

- mzXML & mzData
- pepXML & protXML
- PEDRo a first shot for Proteomics data model (Proteomics Experiment Data Repository) (Taylor et al. 2003)
- MIAPE, PSI-OM, AnalysisXML, Fuge – OM: in development

SBEAMS – Proteomics
Current Status

- Still under development but being used regularly by several researchers
- Current installations: ISB internal, MacroGenics, SBRI, UW, Zurich

- Current stats for ISB instance:

380 experiments (samples)	13.4 M MS/MS spectra
7100 MS runs	25 M SEQUEST searches
8.1 M biosequences	225 M search_hits (possible peptides)
125 GB database	8 x 1.5 GHz, 8 GB RAM, 1 TB disk

SBEAMS – Proteomics
Accessing the System (ISB internal site)

- http://db.systemsbiology.net/ and click on SBEAMS (SSL)

  or just

- https://db.systemsbiology.net/sbeams/
- Access is via SSL from outside the firewall
- Log on with your ISB username and either Windows or UNIX password or else a special account needs to be set up for you

- Test Drive at http://www.sbeams.org/sbeams/

How Can I Use It If Not at ISB?
Installing SBEAMS at another site

Requirements:

- SBEAMS Application Server
  - Perl 5.6+ required
  - Web server required
  - Developed under Linux + Apache
  - Anecdotes of running it on Windows exist but not yet at ISB
- RDBMS (separate machine recommended but not required)
  - Developed on SQL Server
  - SBEAMS Core tested on MySQL and PostgreSQL
  - Proteomics module has not. Could be ported with some effort
- Database programmer
  - Effort in getting it installed at your site should not be underestimated
  - And it will required on going management and development

Download It and Install It:

- http://www.sbeams.org/

Outline

Topics

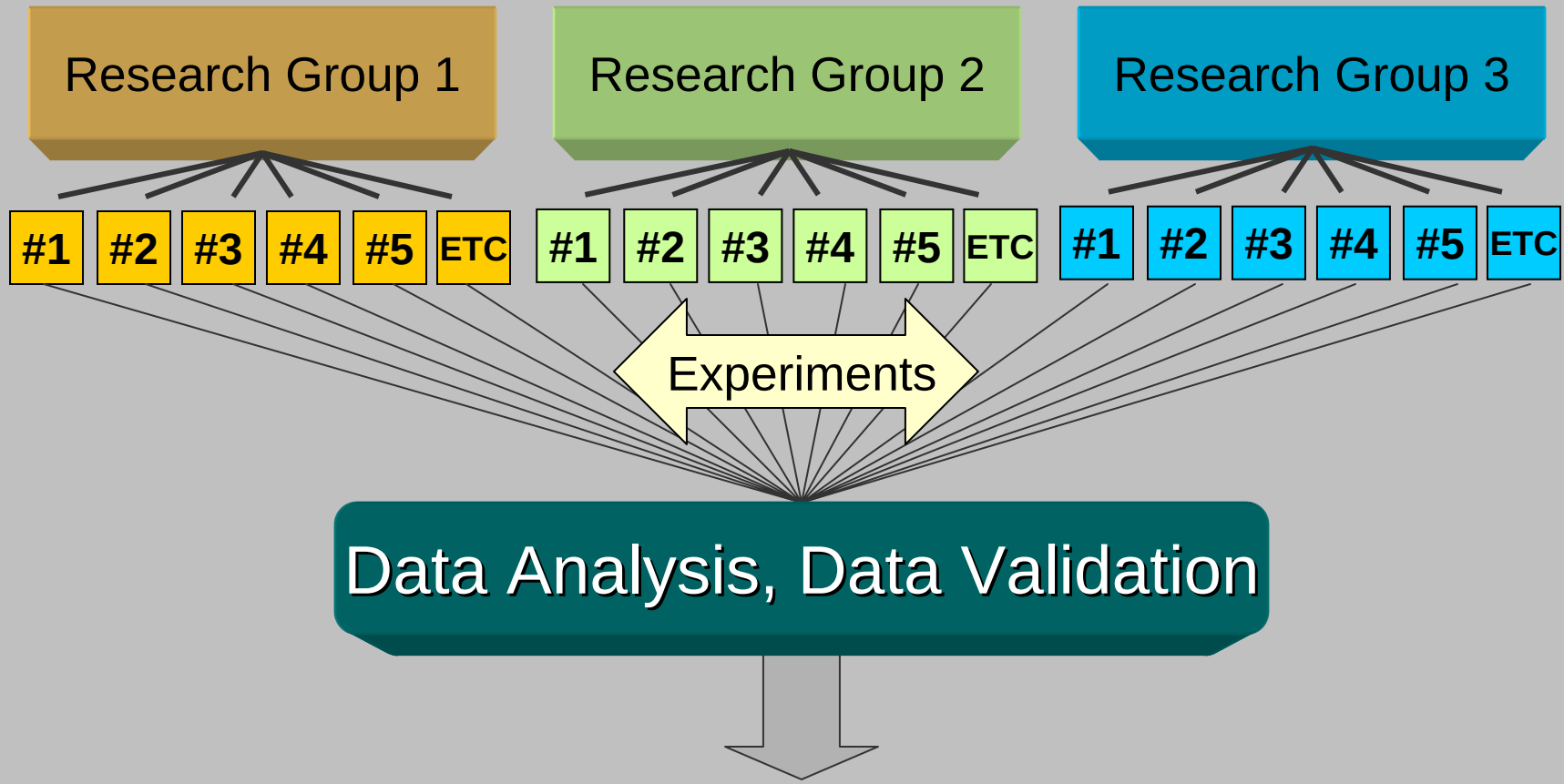
- Introduction to SBEAMS
- SBEAMS – Proteomics
- PeptideAtlas
- Tutorial and Exercises

PeptideAtlas
Background

- There are many shotgun proteomic datasets of which only a small part of the information potential has been used
  - Only a limited set of proteins were of interest
  - Analysis software is still far from optimal
  - Experiment did not properly address hypothesis and is unpublished

- What further benefit can be extracted from a large group of heterogeneous experiments?

PeptideAtlas
Combining Many Heterogeneous Experiments



PeptideAtlas
What Is It?

- PeptideAtlas is the integration of a large number of uniformly processed tandem mass spec experimental results into a master list of observed peptides mapped to the genome

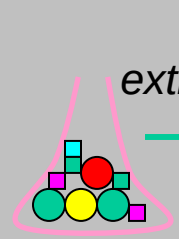
- Currently includes ~250 experiments from:
  - Aebersold lab
  - ISB Proteomics Facility (including data from external clients)
  - NHLBI Consortium members (Yale: Williams, JHU: Pandey)
  - Data from the Open Proteomics Database (OPD@UT: Marcotte)
  - Other contributors (Reising, Gygi, Haynes, Hogue, Conrads..)

- ISB is well suited to start this because of the large amount of in-house data and the general lack of publicly available data

PeptideAtlas
Why?

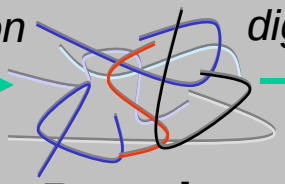
- Genome Annotation:
  - Validating “predicted” proteins
  - Validating intron/exon boundaries and alternative splice forms
  - Validating the reference protein databases (e.g., we find many peptides that don’t map to Ensembl)
- Experiment Planning:
  - Which proteins & peptides are observable with MS/MS
  - Targeted proteomics via inclusion lists
- Data Analysis Aid:
  - Use the web UI to examine whether a protein/peptide in your experiment is already in the PeptideAtlas, which samples, how often, etc.
  - Faster MS/MS analysis using spectrum libraries
- Data Mining:
  - Exploring which peptides are seen and which are not
  - Exploring MS/MS spectral patterns
- Defining the (MS/MS observable) Proteome

From Peptides to Genome Annotation



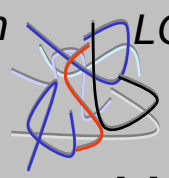
Sample

extraction



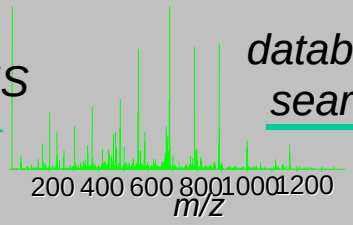
Proteins

digestion



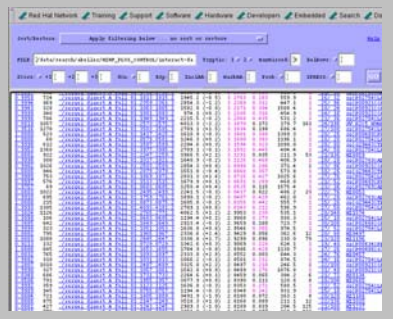
Peptides

LC-MS/MS



Mass Spectrum

database search



Peptides

statistical filtering

Spectrum	Peptide	Probability
Spectrum 1	LGEYGH	1.0
...	...	...
Spectrum N	EIQKKF	0.3

SBEAMS

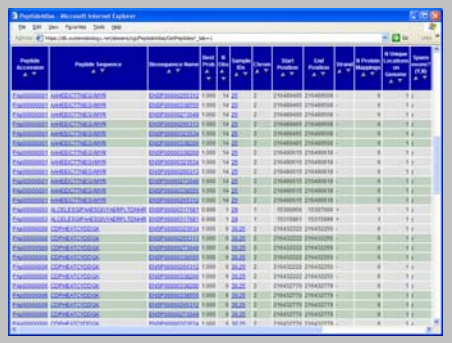
BLAST protein database

Map to genome

Peptide	...	Chrom	Start_Coord	End_Coord	...
PAp00007336	...	X	132217318	132217368	...
...	...	...	...	...	...

Genome Browser

visualization



PeptideAtlas Database

http://www.peptideatlas.org/

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ATLAS DATA:
Data Repository
PeptideAtlas Builds
Search Database
Contribute Data
Genome Browser Setup
GLOSSARY/TERMS:
Atlas nomenclature
SGD nomenclature
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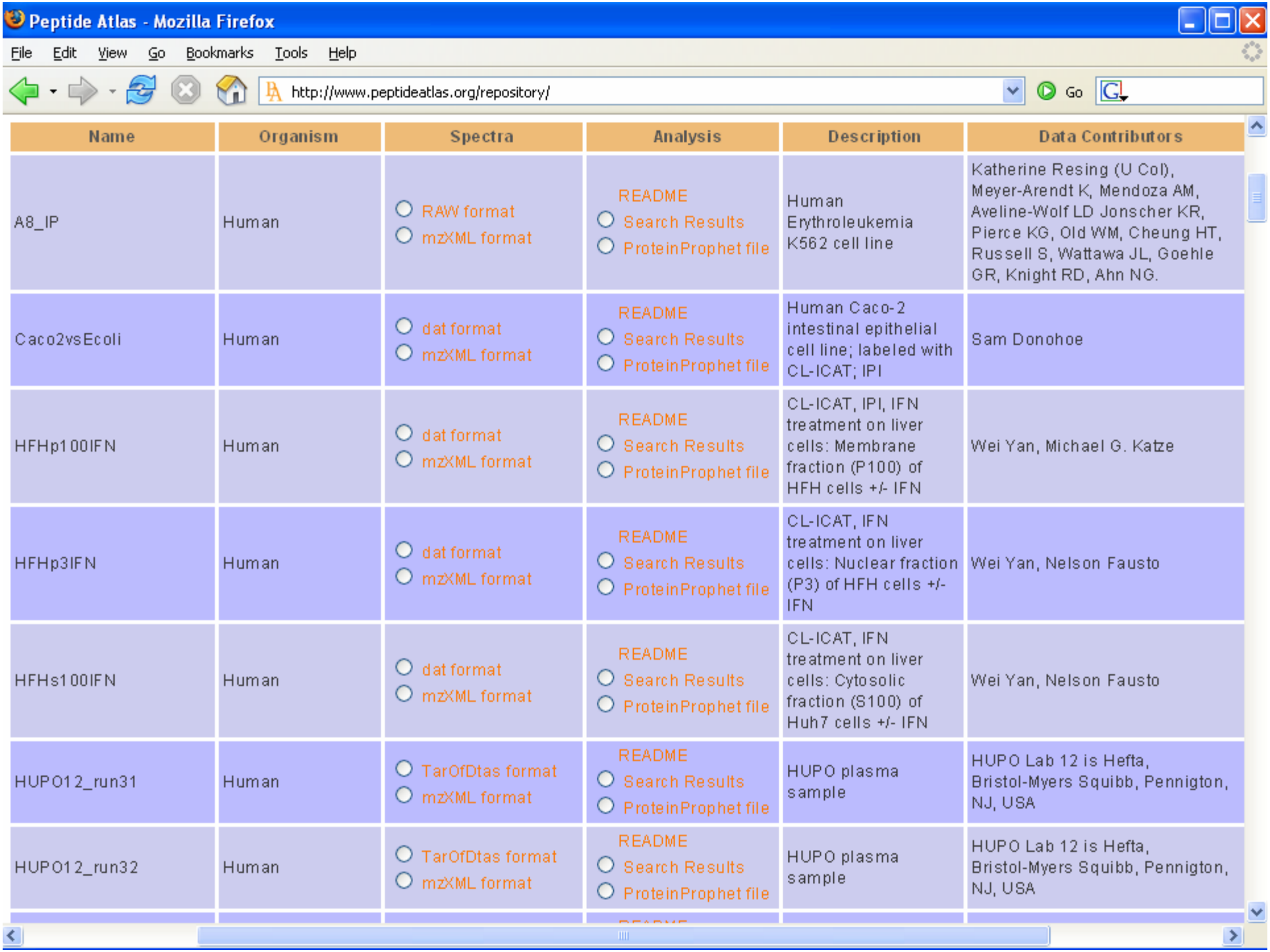
PeptideAtlas Data Contributors
The PeptideAtlas team would like to thank all of the contributors who have made their data, both published and still unpublished, available to us for this project. For additional listings, please see repository.
Published Data
Name
Cell Type
Publication
Priska von Haller
Human Jurkat T-cell lipid raft associated proteins
von Haller et al. 2003, Mol Cell Proteomics, 2, 428
von Haller et al. 2003, Mol Cell Proteomics. 2003 Jul;2(7):426-7.
Phil Hardwidge, Brett Finlay
Human Caco-2 intestinal epithelial cell line
Hardwidge PR, et al. 2004 J Biol Chem., 279(19):20127-36.
Jeff Ranish
Human Hela nuclear extract
Himeda CL et al., 2004., Mol Cell Biol.;24(5):2132-43.
Michael Wright
Human prostate cancer cell line: LNCaP (membrane)
Wright ME et al. 2003. Genome Biol.;5(1):R4.
Wei Yan (ISB), Michael G. Katze (UW), Nelson Fausto (UW)
Human liver carcinoma cell line (Huh7 and HFH cells)
Yan, W. et al. (2004) Genome Biology 2004, 5:R54;
Yan, W. et al. (2004) Mol Cell Proteomics. 2004 Jul 21
Mark Carlson (UT, Austin), John Prince (UT), R Wang (UT), P Lu (UT),
Human SiHa cell line and SqCC cell lines;
Prince et al. (2004) Nature Biotechnology,



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Caco2vsEcoli	Human	dat format mzXML format	README Search Results ProteinProphet file	Human Caco-2 intestinal epithelial cell line; labeled with CL-ICAT; IPI	Sam Donohoe
HFHp100IFN	Human	dat format mzXML format	README Search Results ProteinProphet file	CL-ICAT, IPI, IFN treatment on liver cells: Membrane fraction (P100) of HFH cells +/- IFN	Wei Yan, Michael G. Katze
HFHp3IFN	Human	dat format mzXML format	README Search Results ProteinProphet file	CL-ICAT, IFN treatment on liver cells: Nuclear fraction (P3) of HFH cells +/- IFN	Wei Yan, Nelson Fausto
HFHs100IFN	Human	dat format mzXML format	README Search Results ProteinProphet file	CL-ICAT, IFN treatment on liver cells: Cytosolic fraction (S100) of Huh7 cells +/- IFN	Wei Yan, Nelson Fausto
HUPO12_run31	Human	TarOfDtas format mzXML format	README Search Results ProteinProphet file	HUPO plasma sample	HUPO Lab 12 is Hefta, Bristol-Myers Squibb, Pennington, NJ, USA
HUPO12_run32	Human	TarOfDtas format mzXML format	README Search Results ProteinProphet file	HUPO plasma sample	HUPO Lab 12 is Hefta, Bristol-Myers Squibb, Pennington, NJ, USA

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Data Repository
PeptideAtlas Builds
Search Database
Contribute Data
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Build type: Any
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SBEAMS - PeptideAtlas 0.23-dev
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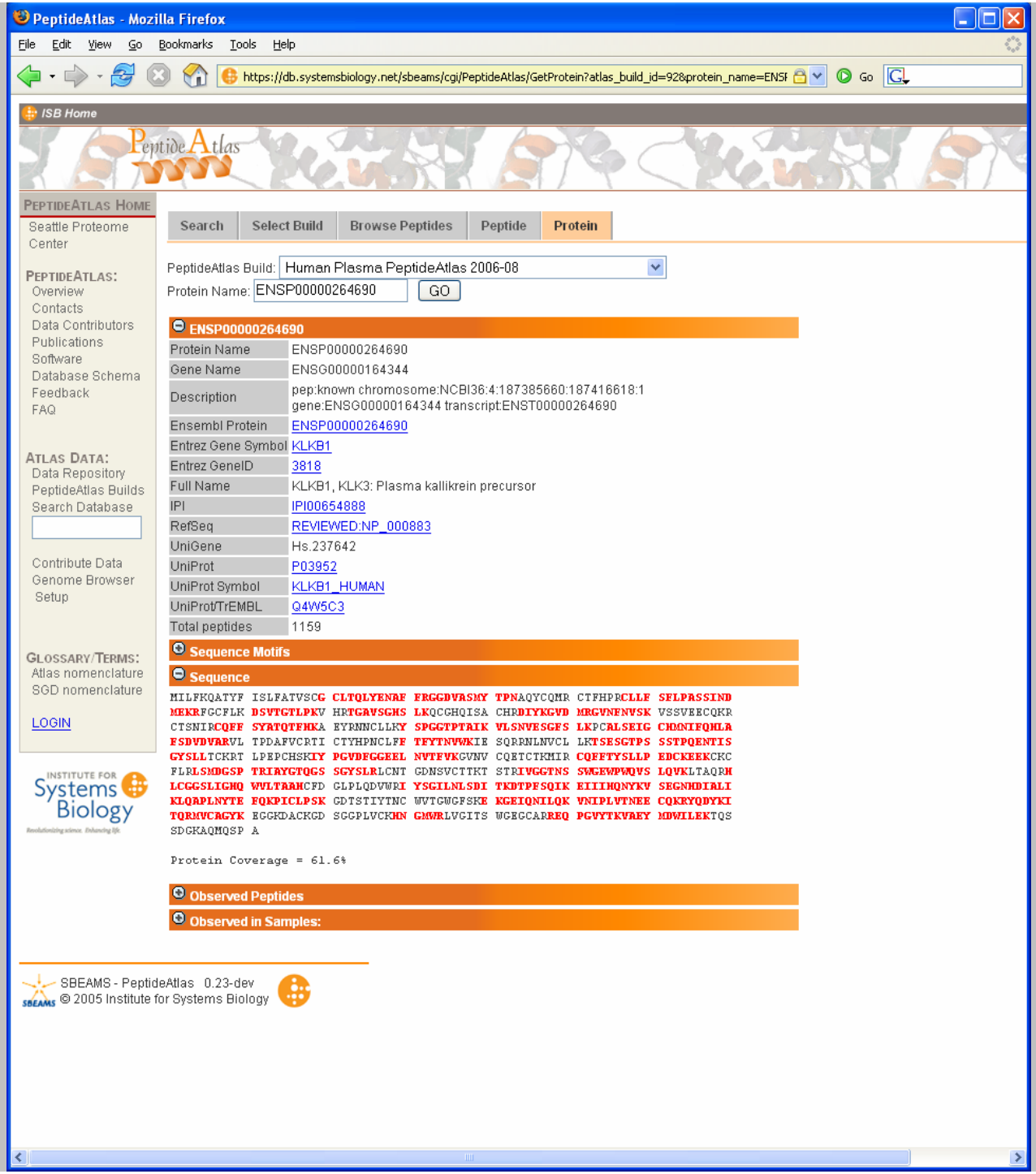
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SGD nomenclature
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Browse Peptides
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RefSeq REVIEWED:NP_000883
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Total peptides 1159
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CTSNIRCQFF SYATQTFHKA EYRNNCLLKY SPGGTPTAIK VLSNVESGFS LKPCALSEIG CHMNIFQHLA
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LCGGSLIGHQ WVLTAAHCFD GLPLQDVWRI YSGILNLSDI TKDTPFSQIK EIIIHQNYKV SEGNHDIALI
KLQAPLNYTE FQKPICLPSK GDTSTIYTNC WVTGWGFSKE KGEIQNILQK VNIPLVTNEE CQKRYQDYKI
TQRMVCAGYK EGGKDACKGD SGGPLVCKHN GMWRLVGITS WGEGCARREQ PGVYTKVAEY MDWILEKTQS
SDGKAQMQSP A
Protein Coverage = 61.6%
Observed Peptides
Observed in Samples:
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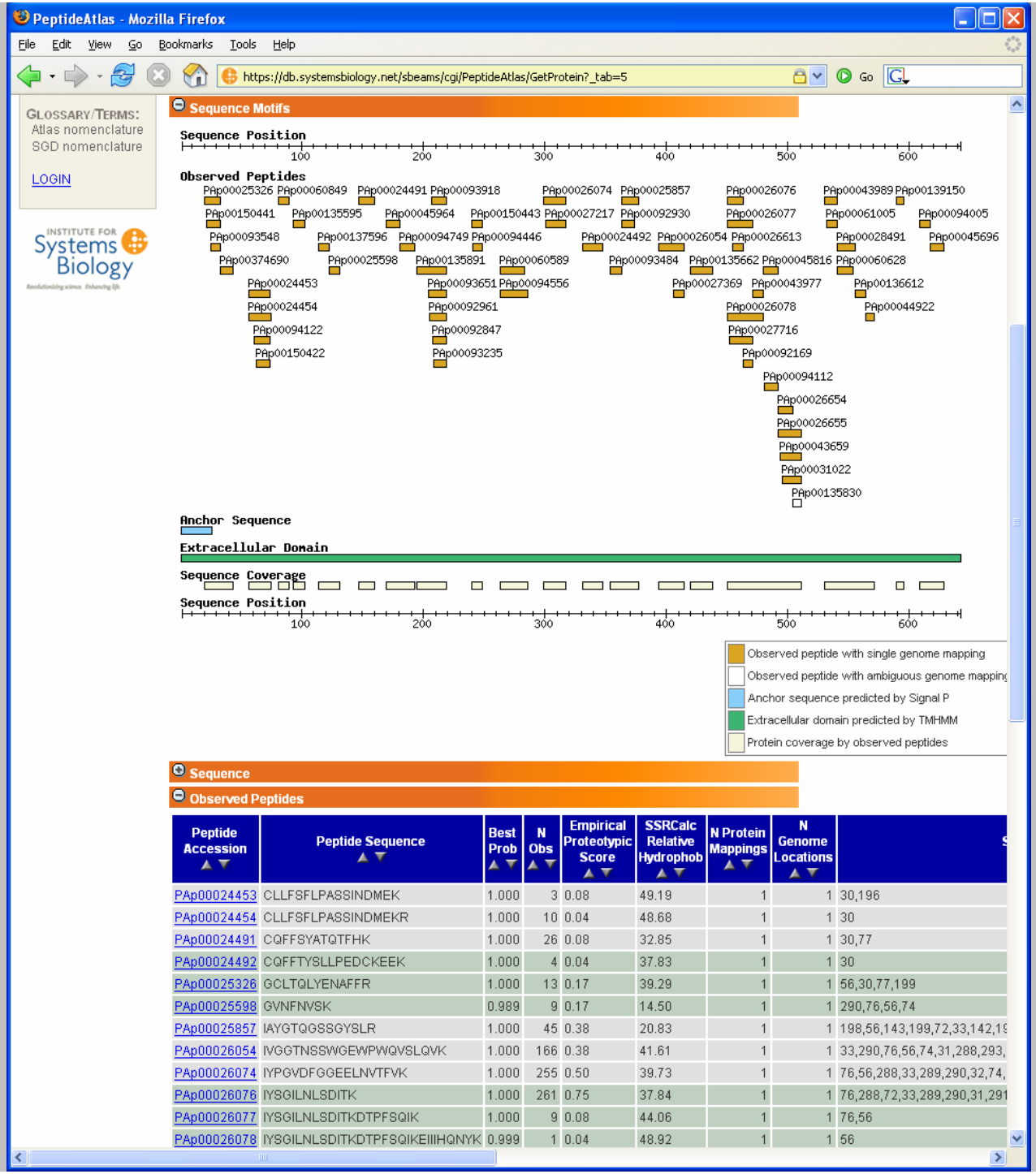

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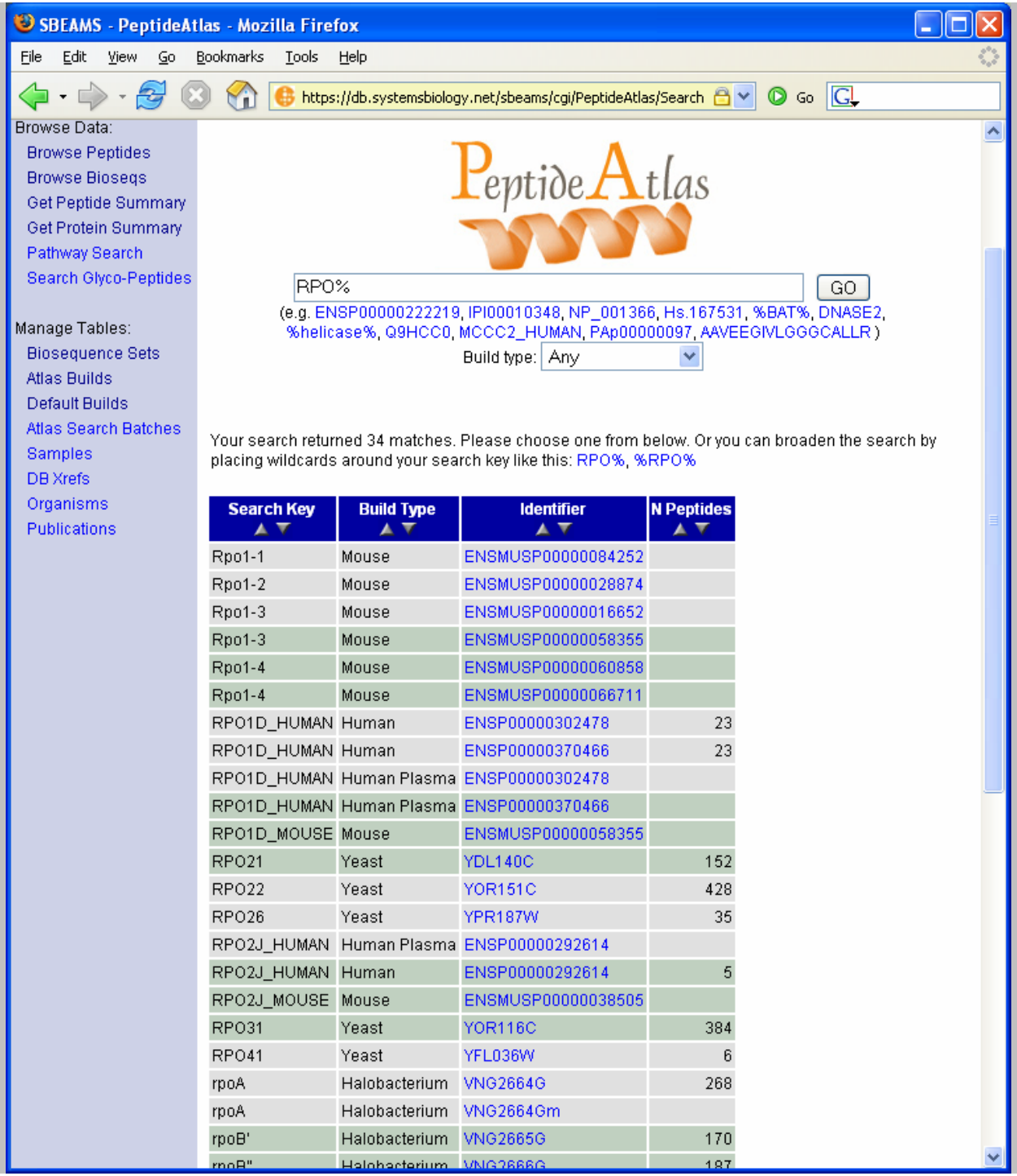
PAp00024491	CQFFSYATQTFHK	1.000	26	0.08	32.85	1	1	30,77
PAp00024492	CQFFTYSLLPEDCKEEK	1.000	4	0.04	37.83	1	1	30
PAp00025326	GCLTQLYENAFFR	1.000	13	0.17	39.29	1	1	56,30,77,199
PAp00025598	GVNFNVSK	0.989	9	0.17	14.50	1	1	290,76,56,74
PAp00025857	IAYGTQGSSGYSLR	1.000	45	0.38	20.83	1	1	198,56,143,199,72,33,142,19
PAp00026054	IVGGTNSSWGEWPWQVSLQVK	1.000	166	0.38	41.61	1	1	33,290,76,56,74,31,288,293,
PAp00026074	IYPGVDFGGEELNVTFVK	1.000	255	0.50	39.73	1	1	76,56,288,33,289,290,32,74,
PAp00026076	IYSGILNLSDITK	1.000	261	0.75	37.84	1	1	76,288,72,33,289,290,31,291
PAp00026077	IYSGILNLSDITKDTPFSQIK	1.000	9	0.08	44.06	1	1	76,56
PAp00026078	IYSGILNLSDITKDTPFSQIKEIIIHQNYK	0.999	1	0.04	48.92	1	1	56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Atlas Builds
Default Builds
Atlas Search Batches
Samples
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Build type: Any
Your search returned 34 matches. Please choose one from below. Or you can broaden the search by placing wildcards around your search key like this: RPO%, %RPO%
Search Key
Build Type
Identifier
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Rpo1-1 Mouse ENSMUSP00000084252
Rpo1-2 Mouse ENSMUSP00000028874
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RPO1D_HUMAN Human ENSP00000302478 23
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RPO1D_MOUSE Mouse ENSMUSP00000058355
RPO21 Yeast YDL140C 152
RPO22 Yeast YOR151C 428
RPO26 Yeast YPR187W 35
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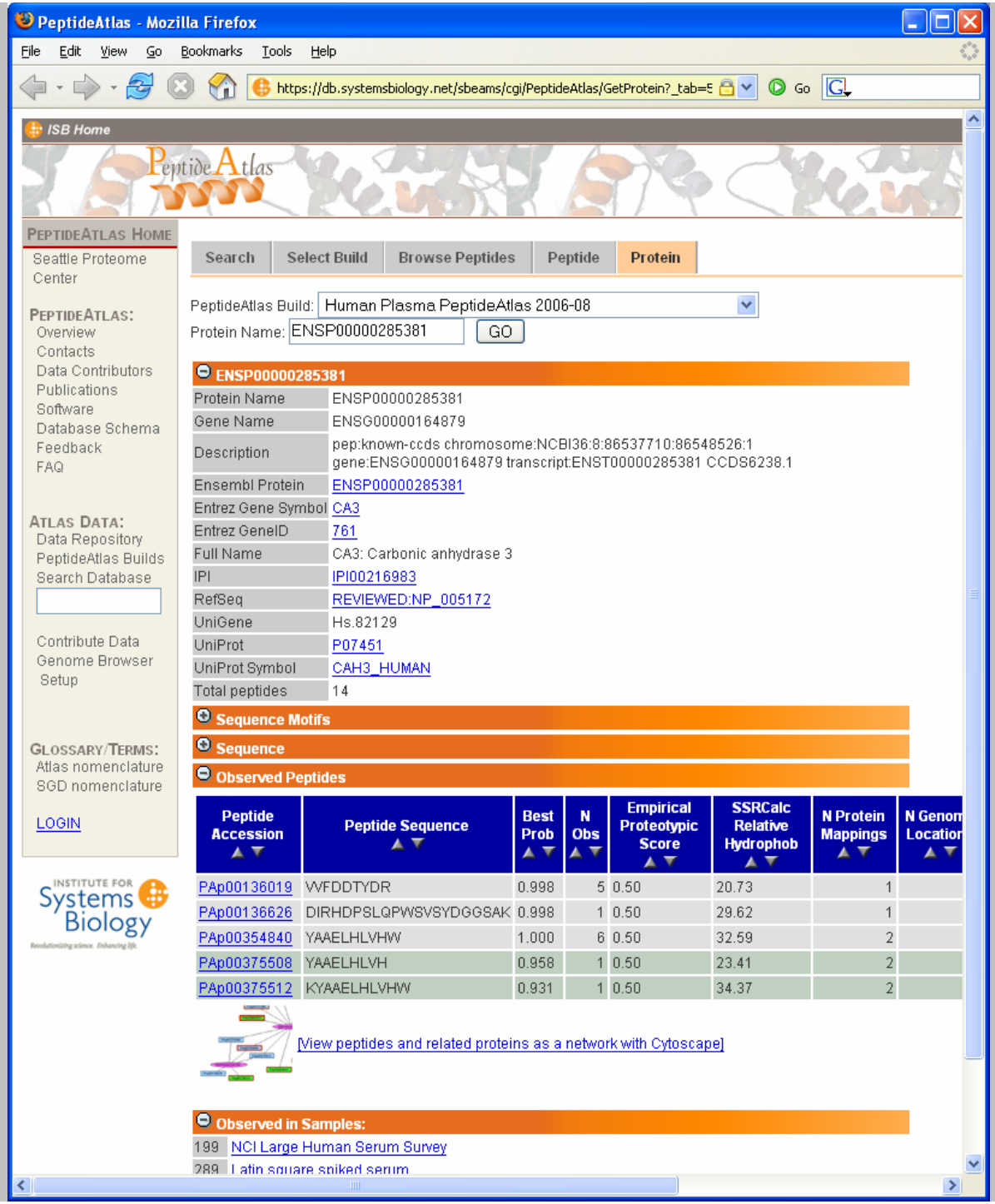
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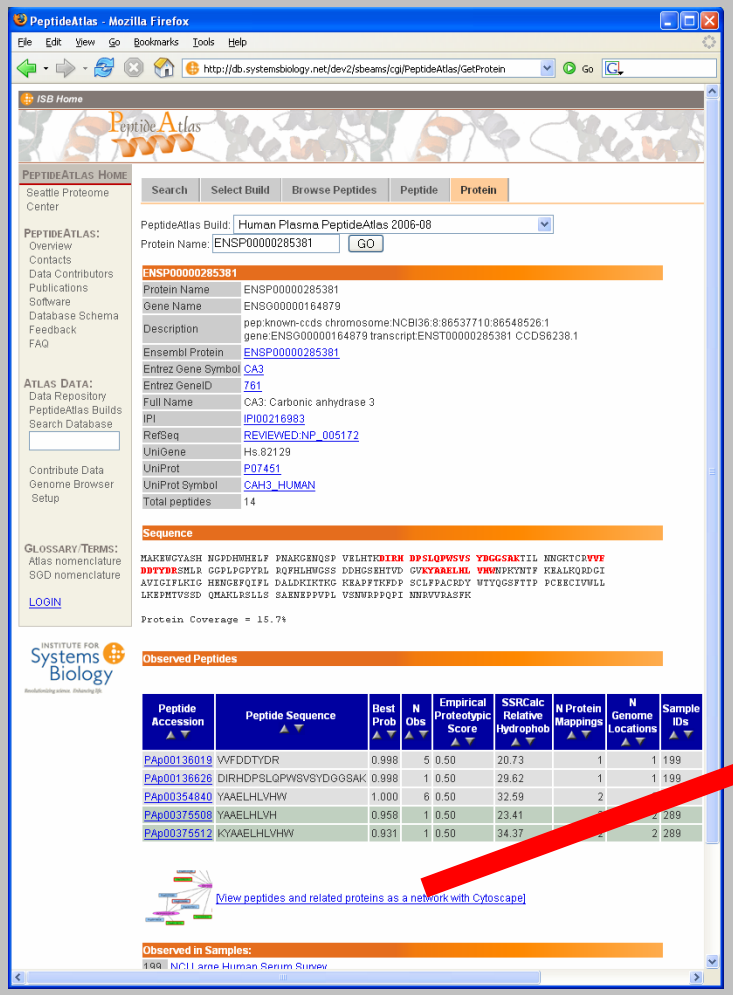
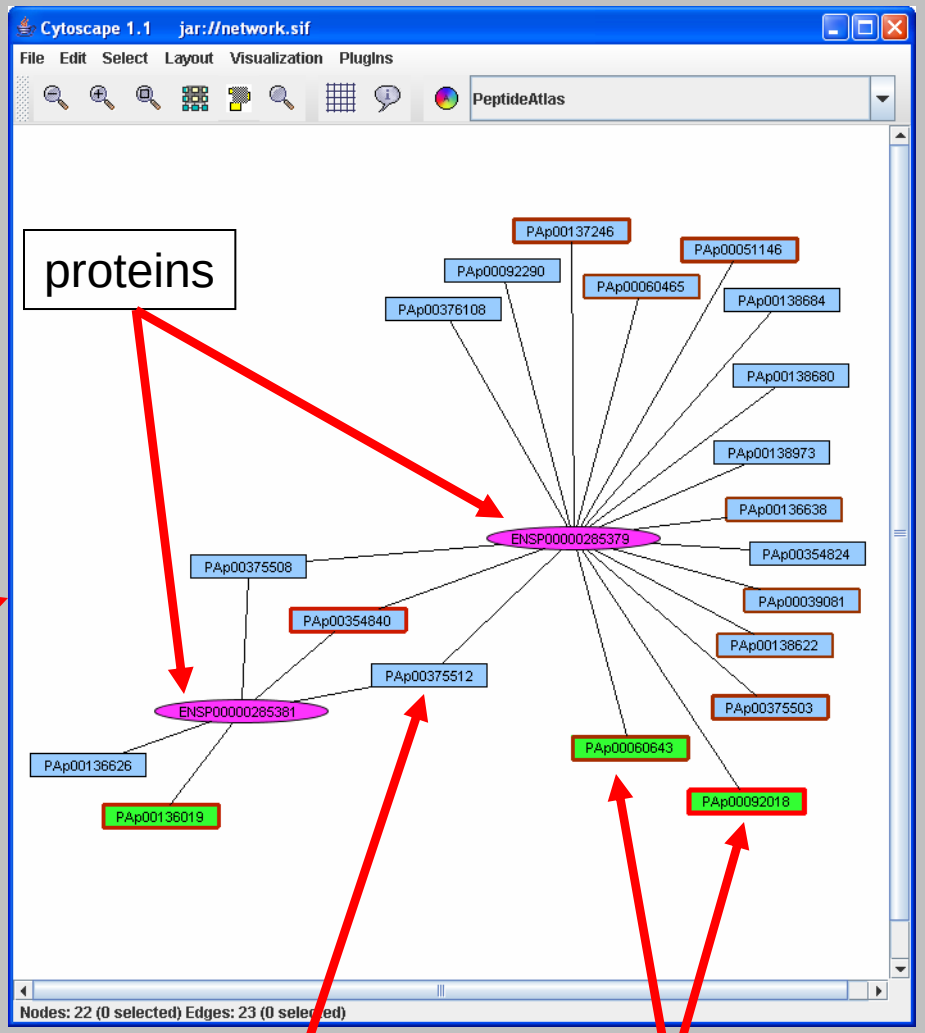
SGD nomenclature
LOGIN
INSTITUTE FOR Systems Biology
Search
Select Build
Browse Peptides
Peptide
Protein
PeptideAtlas Build: Human Plasma PeptideAtlas 2006-08
Protein Name: ENSP00000285381
GO
ENSP00000285381
Protein Name ENSP00000285381
Gene Name ENSG00000164879
Description pep:known-ccds chromosome:NCBI36:8:86537710:86548526:1 gene:ENSG00000164879 transcript:ENST00000285381 CCDS6238.1
Ensembl Protein ENSP00000285381
Entrez Gene Symbol CA3
Entrez GeneID 761
Full Name CA3: Carbonic anhydrase 3
IPI IPI00216983
RefSeq REVIEWED:NP_005172
UniGene Hs.82129
UniProt P07451
UniProt Symbol CAH3_HUMAN
Total peptides 14
Sequence Motifs
Sequence
Observed Peptides
Peptide Accession
Peptide Sequence
Best Prob
N Obs
Empirical Proteotypic Score
SSRCalc Relative Hydrophob
N Protein Mappings
N Genom Location
PAp00136019 VVFDDTYDR 0.998 5 0.50 20.73 1
PAp00136626 DIRHDPSLQPWSVSYDGGSAK 0.998 1 0.50 29.62 1
PAp00354840 YAAELHLVHW 1.000 6 0.50 32.59 2
PAp00375508 YAAELHLVH 0.958 1 0.50 23.41 2
PAp00375512 KYAAELHLVHW 0.931 1 0.50 34.37 2
[View peptides and related proteins as a network with Cytoscape]
Observed in Samples:
199 NCI Large Human Serum Survey
289 Latin square spiked serum

PeptideAtlas protein view page



Cytoscape view of proteins & peptides

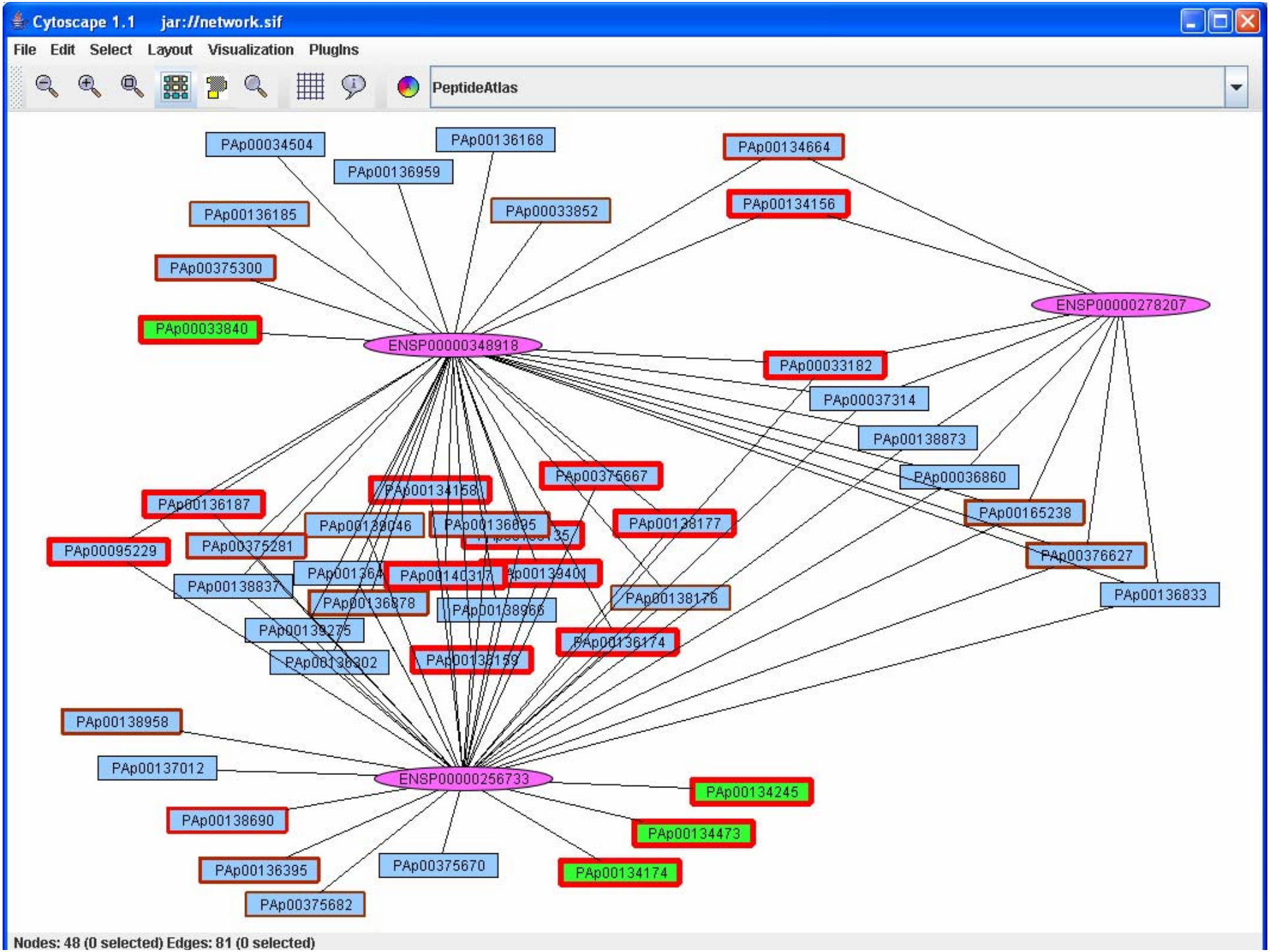


ambiguously mapped peptide

proteotypic peptides

$N_{prot} = 1$ $N_{obs} \geq 1$

EPS > 0.3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PeptideAtlas
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PAp00036860
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PAp00136187
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PAp00138177
PAp00095229
PAp00375281
PAp00376627
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PAp00136174
PAp00138302
PAp00138159
PAp00138958
PAp00137012
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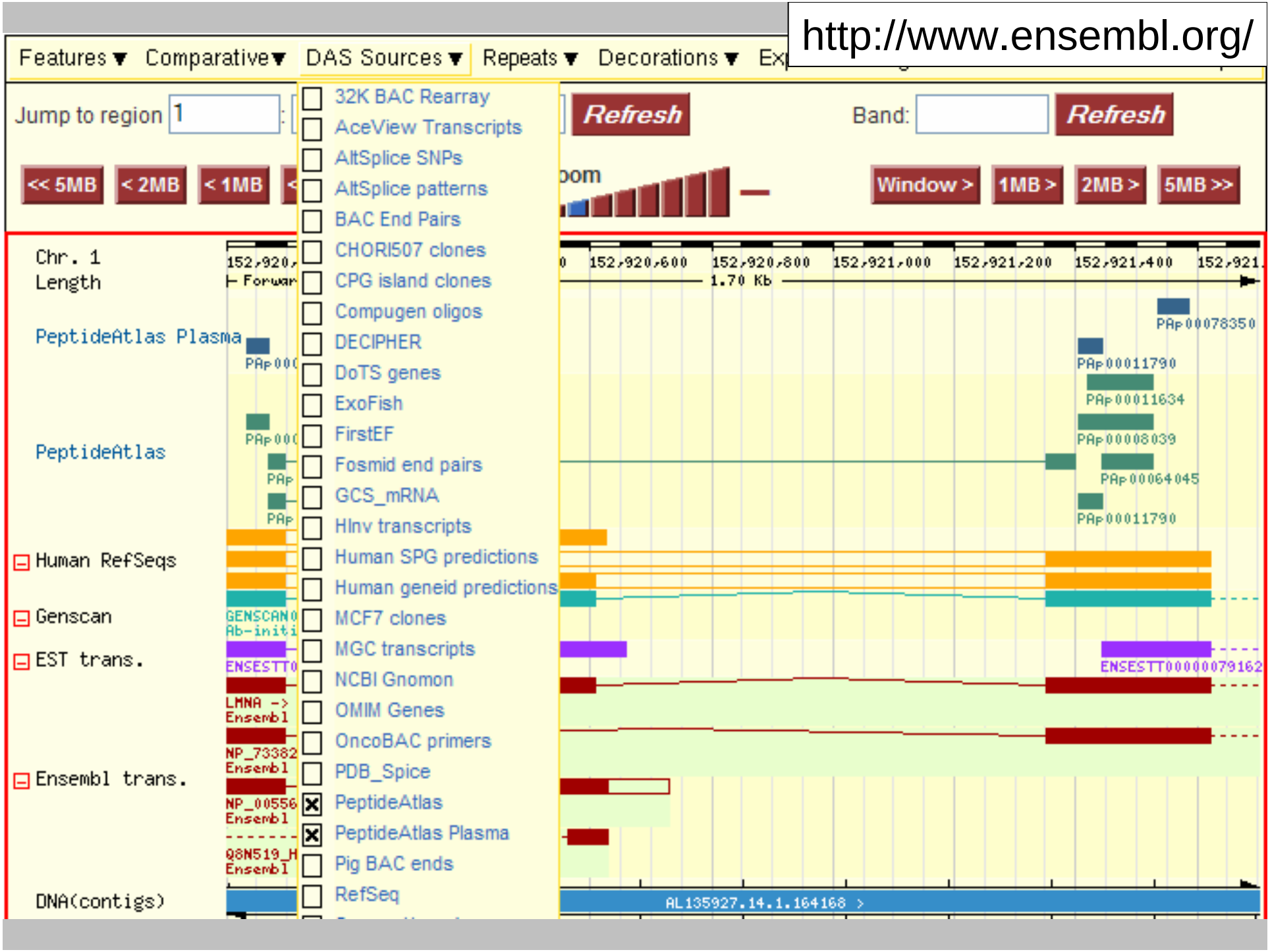
Nodes: 48 (0 selected) Edges: 81 (0 selected)


http://www.ensembl.org/
Features
Comparative
DAS Sources
Repeats
Decorations
Jump to region
1
Refresh
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32K BAC Rearray
AceView Transcripts
AltSplice SNPs
AltSplice patterns
BAC End Pairs
CHORI507 clones
CPG island clones
Compugen oligos
DECIPHER
DoTS genes
ExoFish
FirstEF
Fosmid end pairs
GCS_mRNA
Hlnv transcripts
Human SPG predictions
Human geneid predictions
MCF7 clones
MGC transcripts
NCBI Gnomon
OMIM Genes
OncoBAC primers
PDB_Spice
PeptideAtlas
PeptideAtlas Plasma
Pig BAC ends
RefSeq
Chr. 1
Length
PeptideAtlas Plasma
PeptideAtlas
Human RefSeqs
Genscan
EST trans.
Ensembl trans.
DNA(contigs)
152,920,600
152,920,800
152,921,000
152,921,200
152,921,400
1.70 Kb
PAp00078350
PAp00011790
PAp00011634
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PAp00064045
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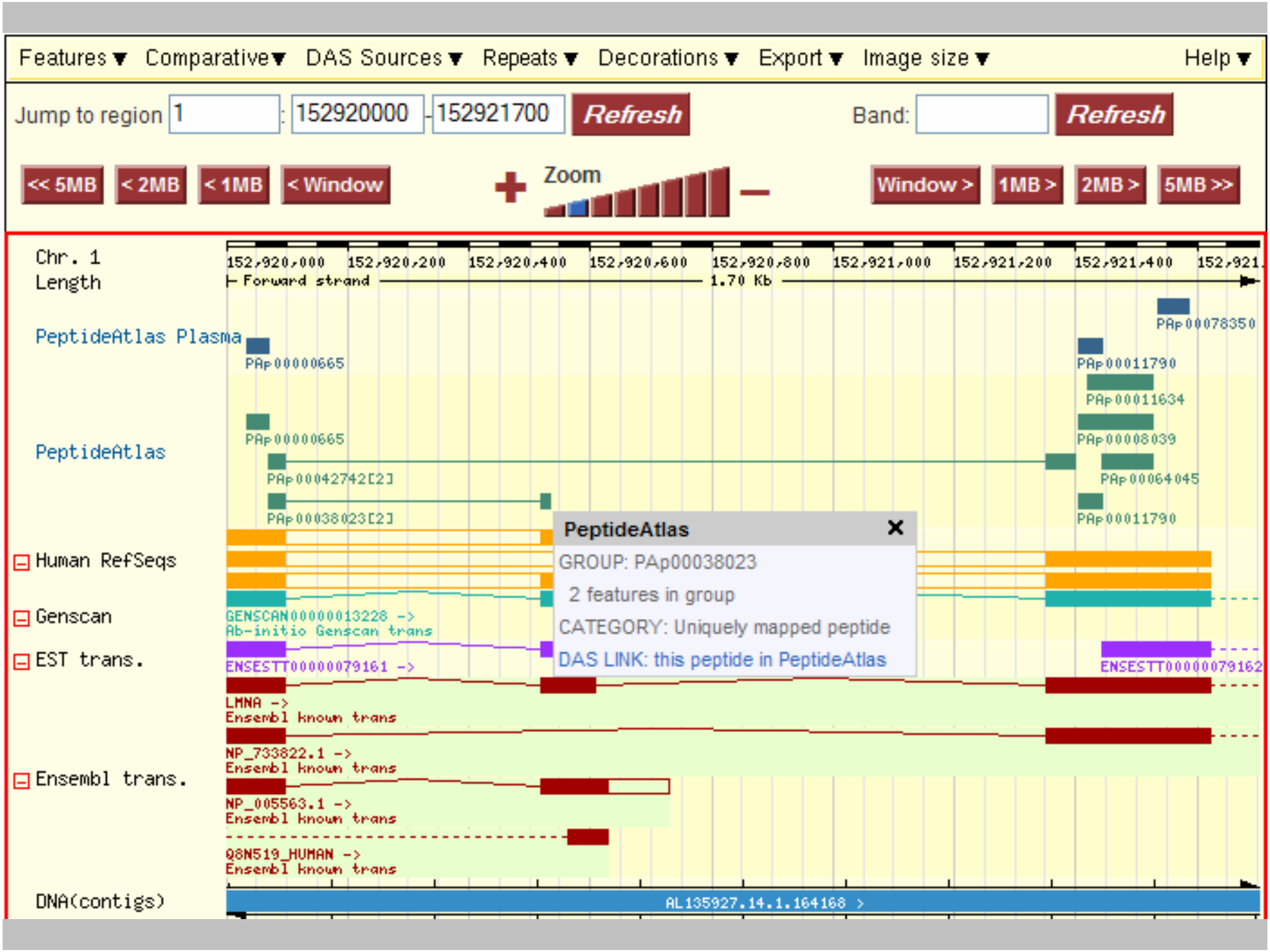
AL135927.14.1.164168 >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Band: Refresh
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Zoom
Window > 1MB > 2MB > 5MB >>
Chr. 1
Length
152,920,000 152,920,200 152,920,400 152,920,600 152,920,800 152,921,000 152,921,200 152,921,400 152,921.
Forward strand
1.70 Kb
PeptideAtlas Plasma
PAp00078350
PAp00000665
PAp00011790
PAp00011634
PeptideAtlas
PAp00000665
PAp00008039
PAp00042742[2]
PAp00064045
PAp00038023[2]
PAp00011790
PeptideAtlas
GROUP: PAp00038023
2 features in group
CATEGORY: Uniquely mapped peptide
DAS LINK: this peptide in PeptideAtlas
Human RefSeqs
Genscan
GENSCAN00000013228 ->
Ab-initio Genscan trans
EST trans.
ENSESTT00000079161 ->
ENSESTT00000079162
LMNA ->
Ensembl known trans
NP_733822.1 ->
Ensembl known trans
Ensembl trans.
NP_005563.1 ->
Ensembl known trans
Q8N519_HUMAN ->
Ensembl known trans
DNA(contigs)
AL135927.14.1.164168 >

PeptideAtlas: Different builds

Build	# Exps	# MS Runs	Searched Spectra	ID P>0.9	Distinct Peptides	Distinct Proteins
Human All	90	1517	3.3 M	334 k	35,391	8000
Drosophila	43	1769	7.5 M	522 k	72 k	9000
Human Plasma	45	38k	13.6 M	1.2 M	15 k	1800
Yeast	46	1326	4.1 M	536 k	35 k	3700
Mouse	6	132	0.3 M	63 k	6 k	1300
Halobacterium	88	497	0.5 M	76 k	12 k	1400

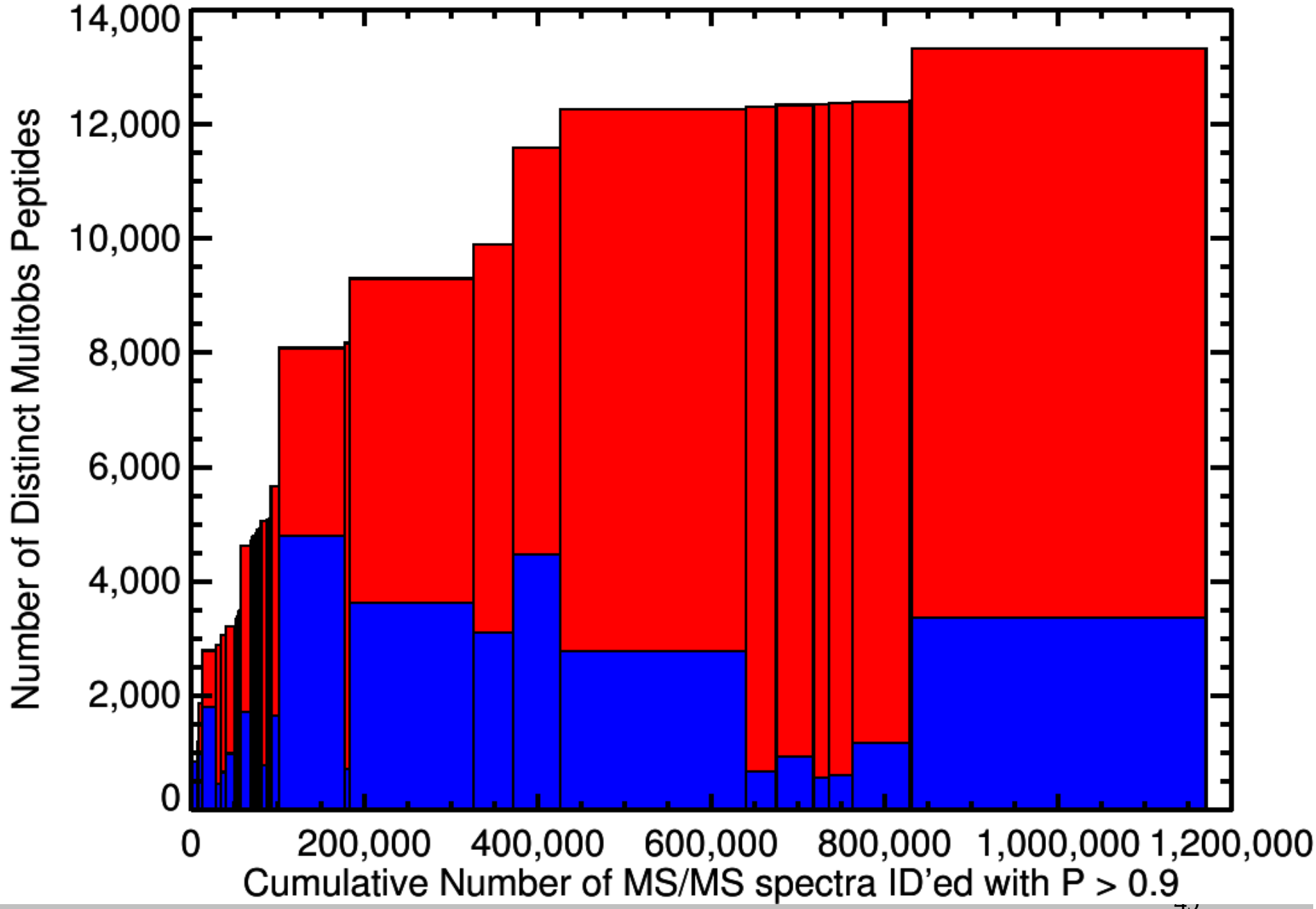
Human Plasma PeptideAtlas

August 2006 Build:

- 45 experiments
- 13.6 million MS/MS spectra searched

Major contributors:

- 2.7 million MS/MS spectra from HUPO PPP datasets
- 1.8 million from NCI (National Cancer Institute)
- 1.9 million from PNNL (Pacific Northwest National Lab)
- 5.1 million from Novartis
- 1.0 million from Cedars-Sinai (Mallick)
- 0.7 million from ISB


14,000
12,000
10,000
8,000
6,000
4,000
2,000
0
Number of Distinct Multobs Peptides
0
200,000
400,000
600,000
800,000
1,000,000
1,200,000
Cumulative Number of MS/MS spectra ID'ed with P > 0.9

Human Plasma PeptideAtlas

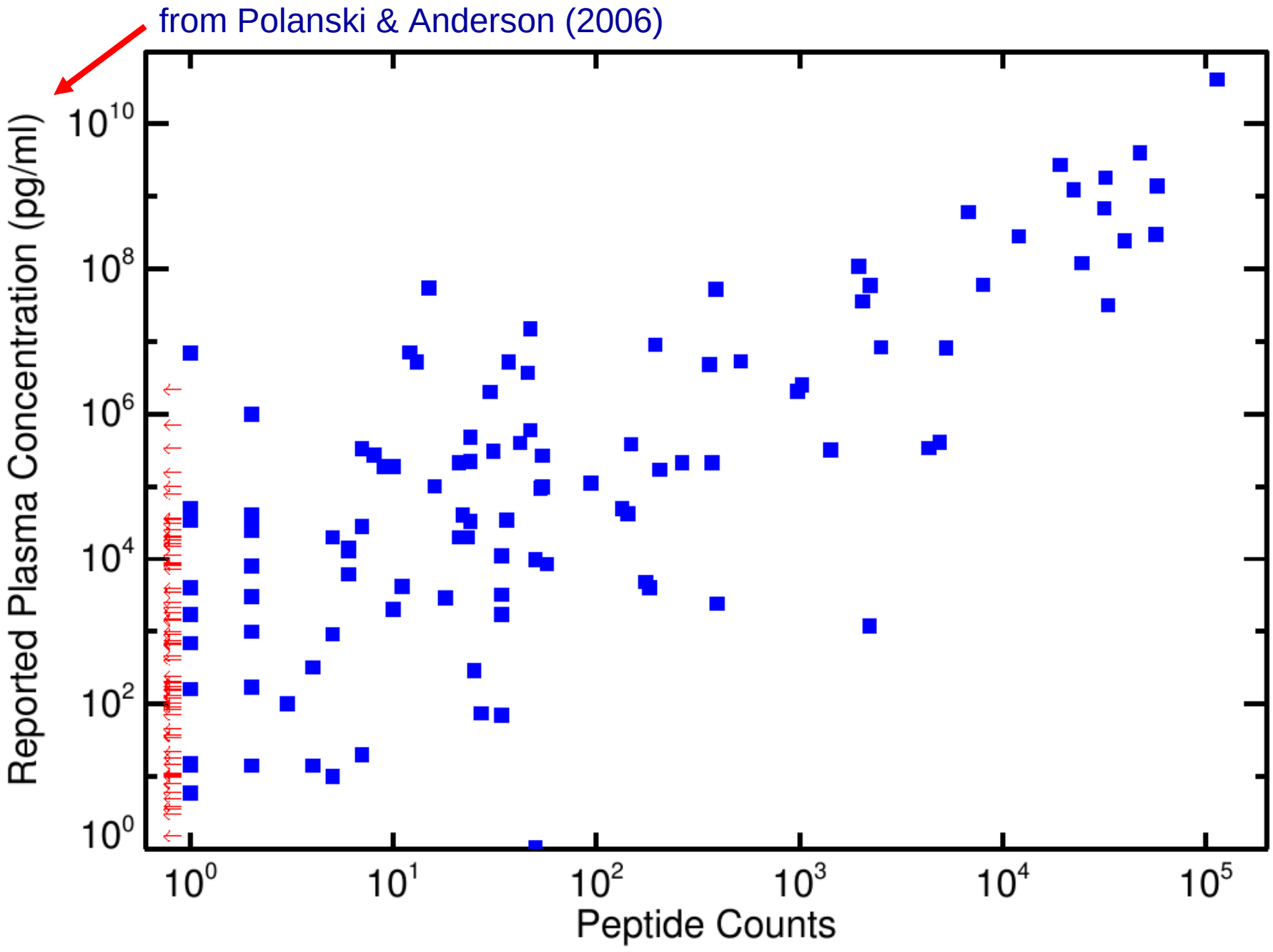
All pep	Multobs	
23.6 k	14.6 k	Total distinct peptides
21.6 k	12.6 k	Total distinct peptides mapping to reference
0.64	0.07	Estimated FDR for peptides
8736	3272	All possible proteins mapped to
5140	1812	Proteins after simple reduction of redundancy
4917	1725	Genes after simple reduction of redundancy

Plasma Proteome State of the Onion

	N Proteins	mappable	Int 3020	Int 889
Shen et al. (2004)	800 / 1682			179
Chan et al. (2004)	1444	1019	257	
Zhou et al. (2004)	210	148	62	
Anderson et al (2004)	1175 (194) (92) (46)	990	316	
Omenn et al. (2005)	3020		-	
Deutsch et al. (2005)	960		479	
States et al. (2006)	889	538		
HPPA 2006-08	1812			346 of 538

Comparison with Polanski & Anderson (2006) "Cancer Proteins"

- 1269 "candidate cancer biomarkers for targeted Proteomics"
- 985 proteins that have useful accession and map to Ensembl
- 192 have a reported plasma protein concentration
- 394 (40%) of those have an entry in Plasma PeptideAtlas
- 112 have concentration and are found in Plasma PeptideAtlas


from Polanski & Anderson (2006)
Reported Plasma Concentration (pg/ml)
10^{10}
10^{8}
10^{6}
10^{4}
10^{2}
10^{0}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
Peptide Counts

PeptideAtlas
Publications

- Initial PeptideAtlas Publication:

  Frank Desiere, Eric W. Deutsch, Alexey I. Nesvizhskii, Parag Mallick, Nichole King, Jimmy K. Eng, ...

  "Integration of Peptide Sequences Obtained by High-Throughput Mass Spectrometry with the Human Genome", Genome Biology 2004, 6:R9

- Human Plasma PeptideAtlas Publication:

  Eric W. Deutsch, Jimmy K. Eng, Hui Zhang, Nichole L. King, Alexey I. Nesvizhskii, ...

  "Human Plasma PeptideAtlas", Proteomics. 2005 Aug;5(13):3497-500

- Yeast PeptideAtlas:

  Nichole L. King, Eric W Deutsch, Jeff Ranish, Alexey I. Nesvizhskii, James S. Eddes, ...

  "Analysis of the S. cerevisiae proteome with PeptideAtlas“, Genome Biology, submitted

- Latest Update:

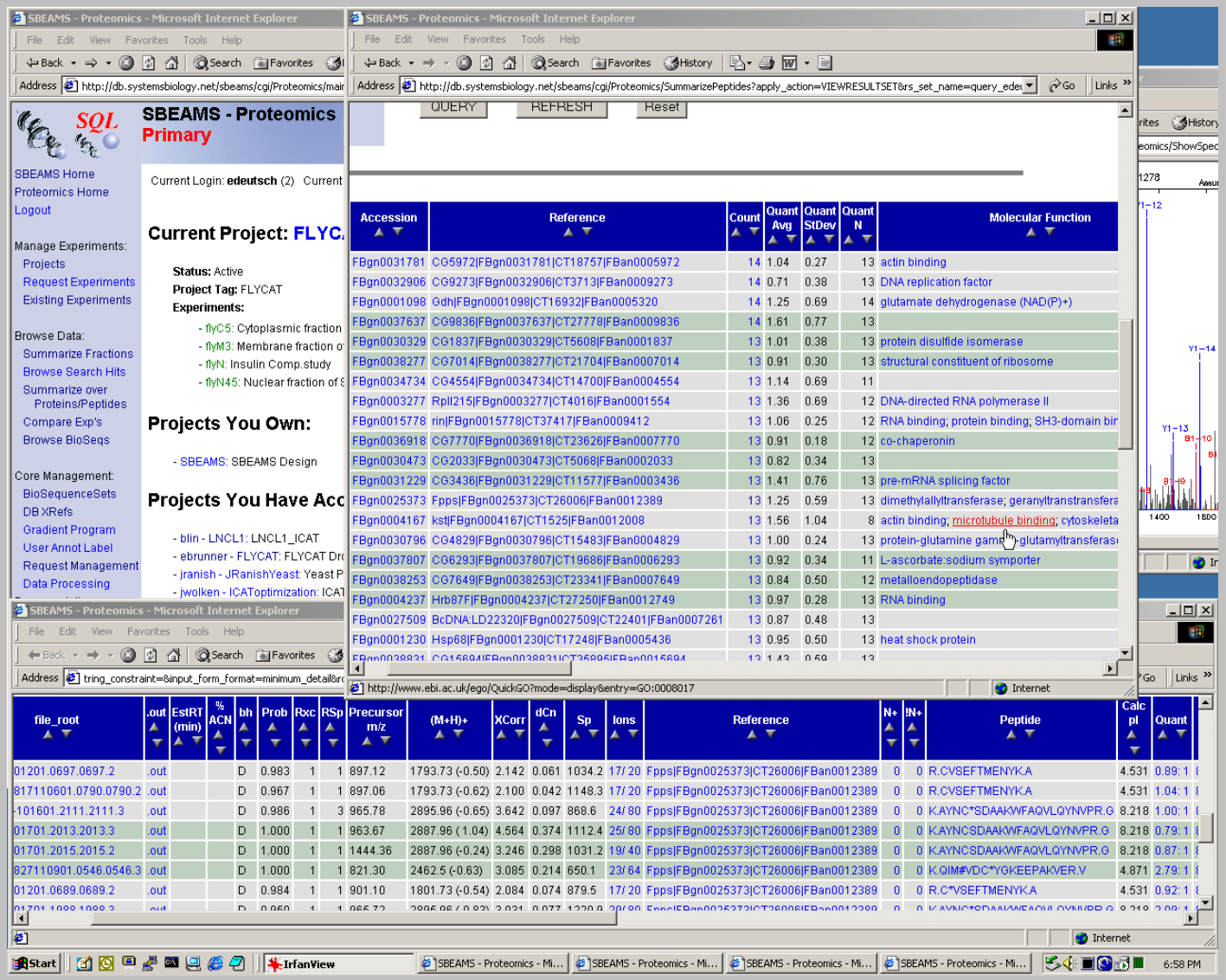
  Frank Desiere, Eric W. Deutsch, Nichole L. King, Alexey I. Nesvizhskii, Parag Mallick, Jimmy Eng, ...

  "The PeptideAtlas Project", Nucleic Acids Research, 2006, 34, D655-D658

PeptideAtlas
How to use it

- Link to / paste in your (human, mouse, drosophila, yeast…) peptides or proteins of interest and see if they have been seen already and in what samples
- Download the PeptideAtlas build results and mine the data
- Contribute your data:
  - Published data. We'll put it up in the repository for others to download
  - Unpublished data. We'll include it in the PeptideAtlas with minimal annotation
  - Human or Mouse data of most interest right now
  - Data from other organisms. We'll take it, esp. Ensembl organisms
  - Preferably the raw files, we'll run it through the pipeline here
- Start your own PeptideAtlas for your favorite organism
  - We plan on releasing all the tools to build your own PeptideAtlas for whatever you want to do

SBEAMS-Proteomics: Tutorial



SBEAMS-Proteomics: Tips and Tricks

- Right click on a link and open it in a new window.
- In list boxes hit the first letter of your item one or more times to jump there.
- In a multi-select list box, hold down CTRL to select/deselect items
- Resultsets are sometimes down below out of sight when a page comes up. Check the up/down scroll bar to see if what you're looking for is just out of sight below.