GREAT LAKES BIOENERGY RESEARCH CENTER

Managing Omics Data at GLBRC

Yury V Bukhman

Bioinfo-Core Workshop, ISMB 2016

U.S. DEPARTMENT OF ENERGY

DOE Bioenergy Research Centers

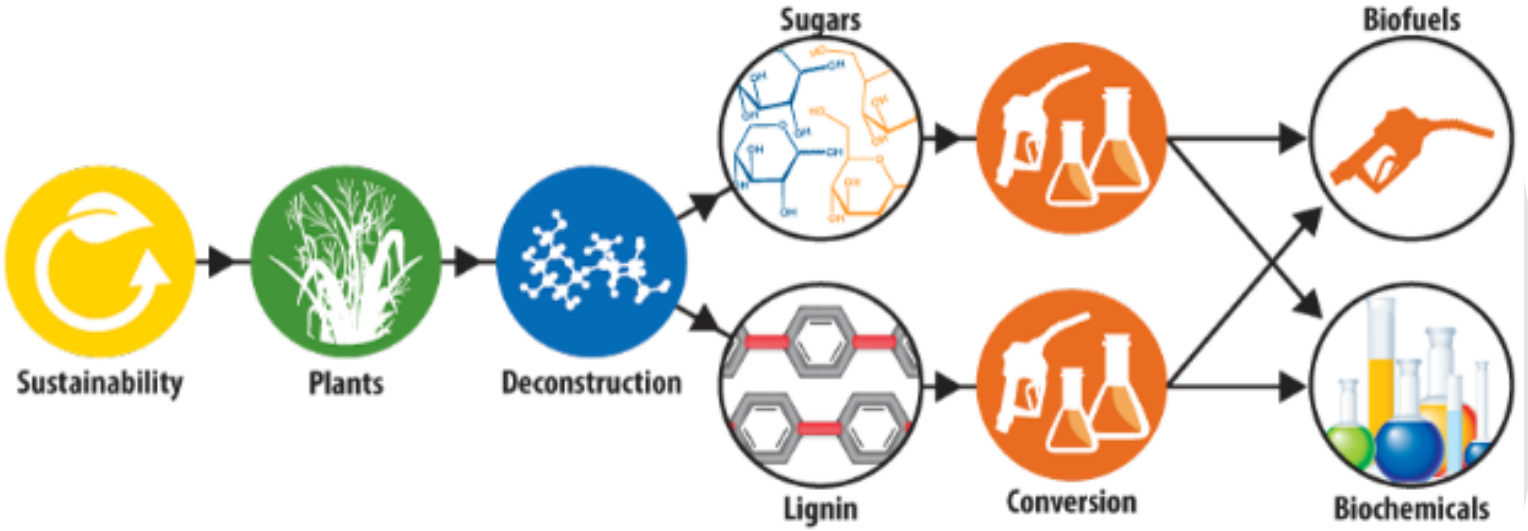
GLBRC = Great Lakes Bioenergy Research Center

- The mission of the Great Lakes Bioenergy Research Center is grand, but simply stated: to perform the basic research that generates technology to convert cellulosic biomass to ethanol and other advanced biofuels.
- DOE-funded, university-based center
- UW – Madison, Michigan State and other partners

GLBRC Structure

- Multiple projects done by academic labs led by professors
- Enabling technologies
  - Core facilities
  - Informatics and Information Technology (IIT)
    - IT
    - LIMS
    - Computational biology
      - Yury the scientist
    - MSU informatics group

GLBRC Data Management Challenges

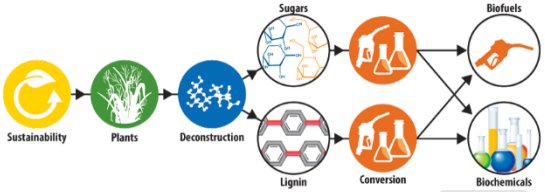


- A wide variety of research projects → many different data types, including omics
- University labs have a high degree of independence, different needs, different practices
- Geographic separation

GLBRC Data Management Solutions

- Each project has a data management plan, reviewed by IIT
  - Several projects have their own databases
- Centralized informatics resources
  - Shared file servers
  - SharePoint
  - LIMS
  - GLOW metadata database
  - GxSeq: Genome Browser, Expression Viewer etc.

Omics Data Flow



Lab samples and materials: field samples, biomass, hydrolysates…

GLBRC LIMS

Sequencing Facilities

bigdata file server

GLOW metadata database

Bioinformatics workflows

GxSeq Genome Suite

GLBRC LIMS

STARLIMS | About | Add/Remove Content | Logout

Dashboard | GLBRC Sample Viewer

Folders List

Search | Export To Excel | Submitter's Lab: GLBRC Product Chain Management

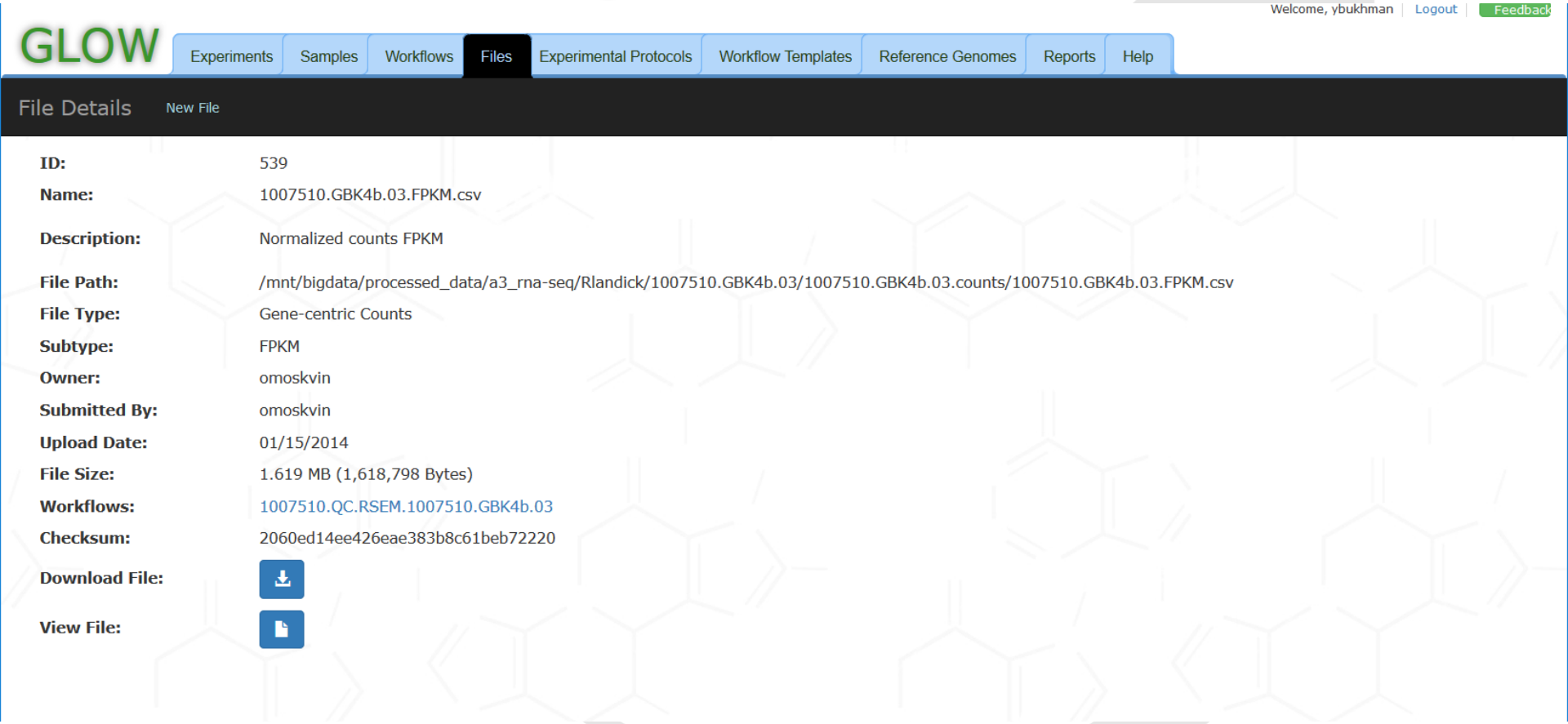
Approval S	Approved	Approved	Status	Folder #	Exp #	Service	Test Plan	Submitted By	Project #	Service Lab	Notes
Releas...	Auto	06/11...	Done	UFS140054	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/11...	Done	UFS140054	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/11...	Done	UFS140053	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/11...	Done	UFS140053	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/11...	Done	UFS140052	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/11...	Done	UFS140052	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/02...	Done	UFS140051	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/02...	Done	UFS140051	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	
Releas...	Auto	06/02...	Done	UFS140050	0	Cell Wall Analyses	Cell Wall Compositio...	RRANATUN...	5.5.2	Cell Wall ...	

Test Results | Attachments

Sample Info	Test	Analyte	Rep	Result	Final	Units	Status	Test Stat	Analyzed Da	Analyzed by	HIGH A	HIGH E	LC	LC
UFS140054001 - FSUWM000000...	Digestibility...	Glucose	1	12.957	12.957	%Yiel...	Done	Done	06/02/2...	CWLIMS				
UFS140054001 - FSUWM000000...	Digestibility...	Glucose	2	9.655	9.655	%Yiel...	Done	Done	06/02/2...	CWLIMS				

Ying Gao, Quansheng Yang, Feiran Yu, LiRong Tao, et al.

GLOW: the File Metadata Database



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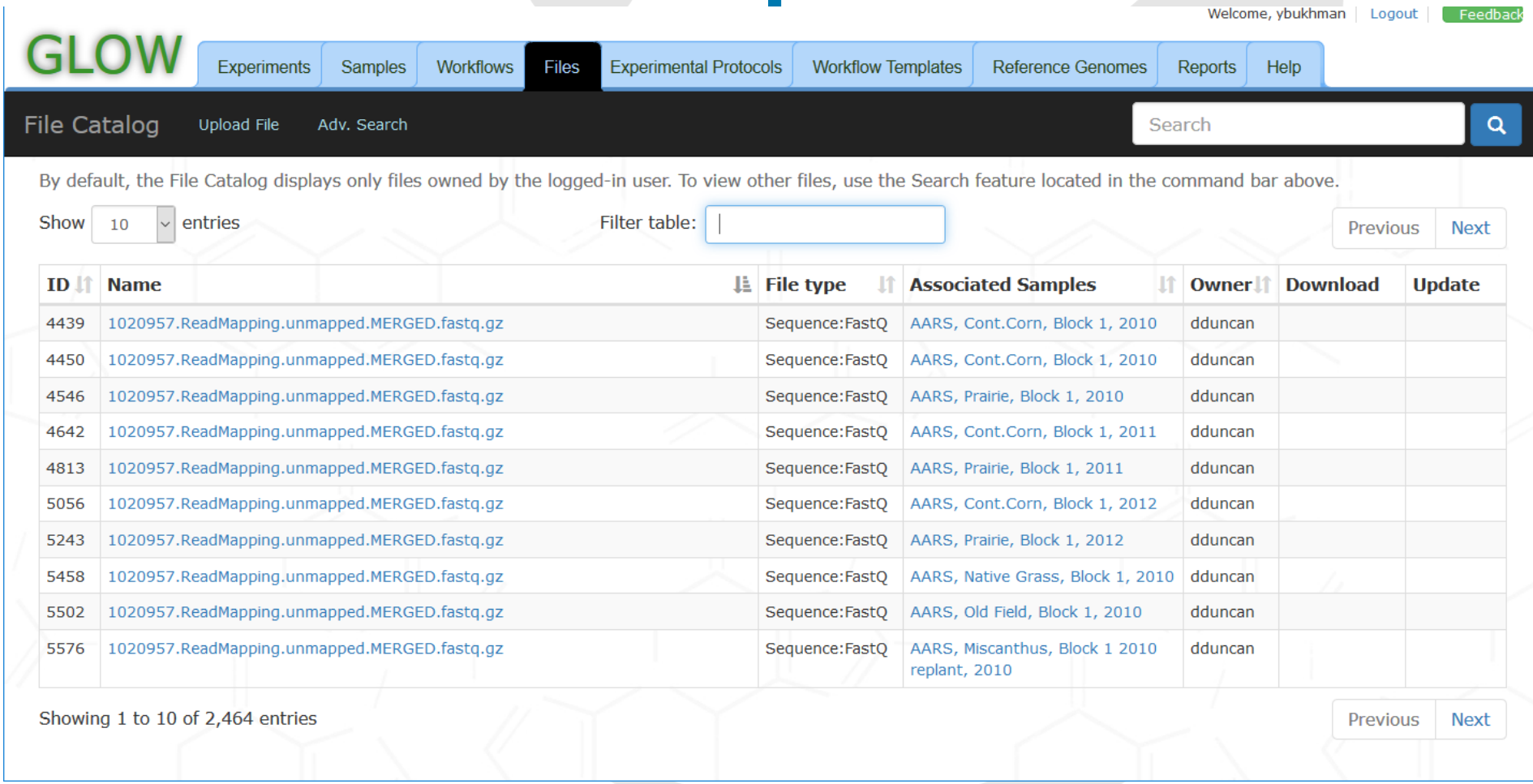
Files are Associated With Samples



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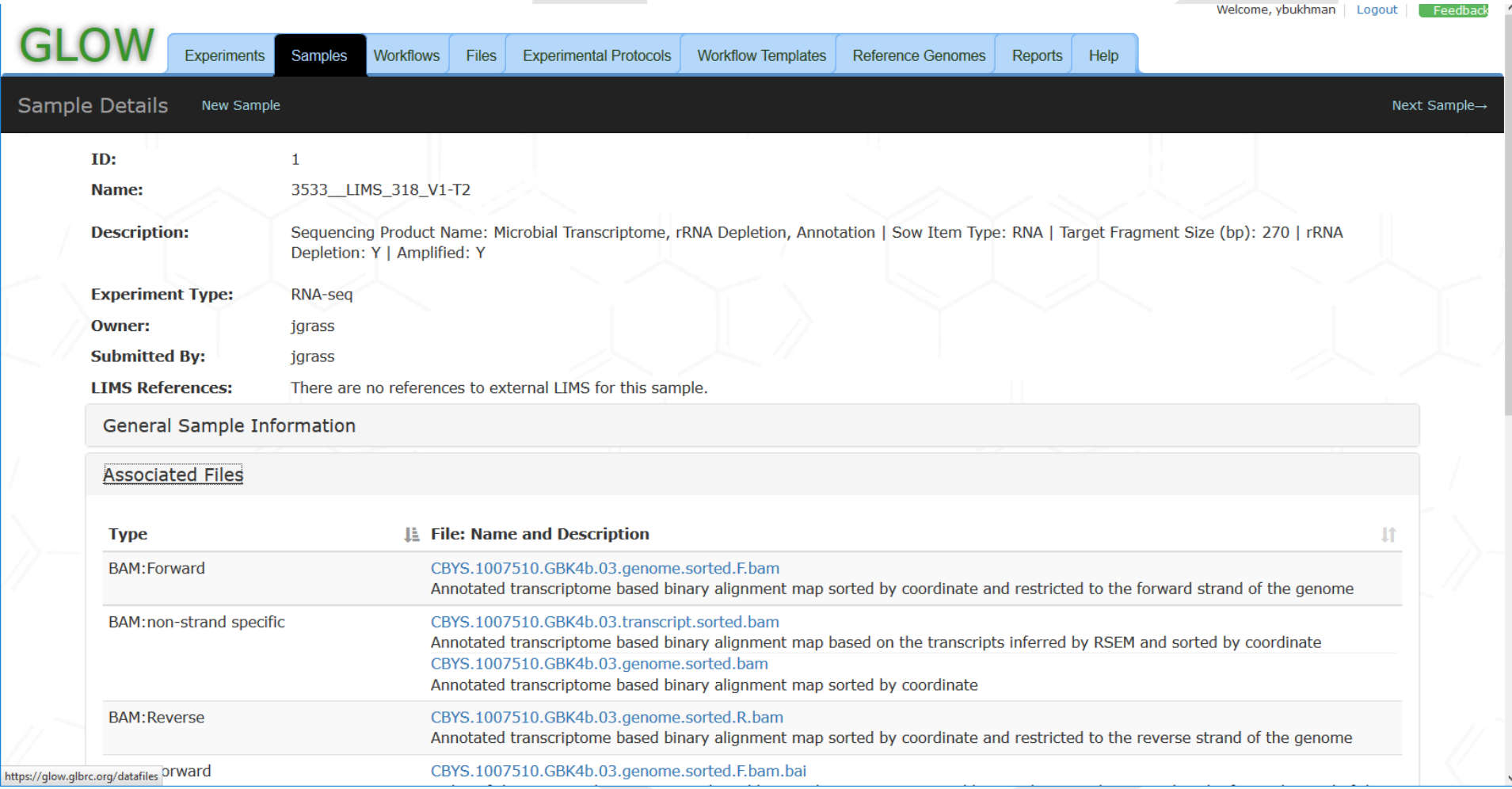
Sample and Its Files



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Samples are Grouped Into Experiment Sets

GLOW

Experiments | Samples | Workflows | Files | Experimental Protocols | Workflow Templates | Reference Genomes | Reports | Help

Experiment Set Details Add To... ←Previous Experiment Set

ID: 1

Name: Escherichia coli K-12 MG1655 3.1.4 Multiomics #1

Description: Project 1007510 uploaded from JGI metadata

Owner: jgrass

Submitted By: jgrass

Samples in this Experiment Set:

Show 10 entries Filter table: Previous Next

ID	Name	Description	Experiment Sets	Experiment Type	Category	Subcategory	Workflows	File Types	Owner	Upload Date	Action
1	3533__LIMS_318_V1-T2	Sequencing Product Name: Mi...	Escherichia coli K-12 MG1655 3.1.4 Multiomics #1;	RNA-seq			1007510.QC.RSEM.1007510.GBK4b.03;	BAM:Forward BAM:Reverse BAM:non-strand specific BAMI:Forward BAMI:Reverse BAMI:non-strand specific Sample-centric Cou...	jgrass	01/14/2014	Add to set • Create workflow •
	3534__LIMS_318_V1-T3	Sequencing	Escherichia coli	RNA-seq			1007510.QC.RSEM.1007510.G	BAM:Forward	jgrass	01/14/2014	Add to set

https://glow.glbrc.org/datafiles

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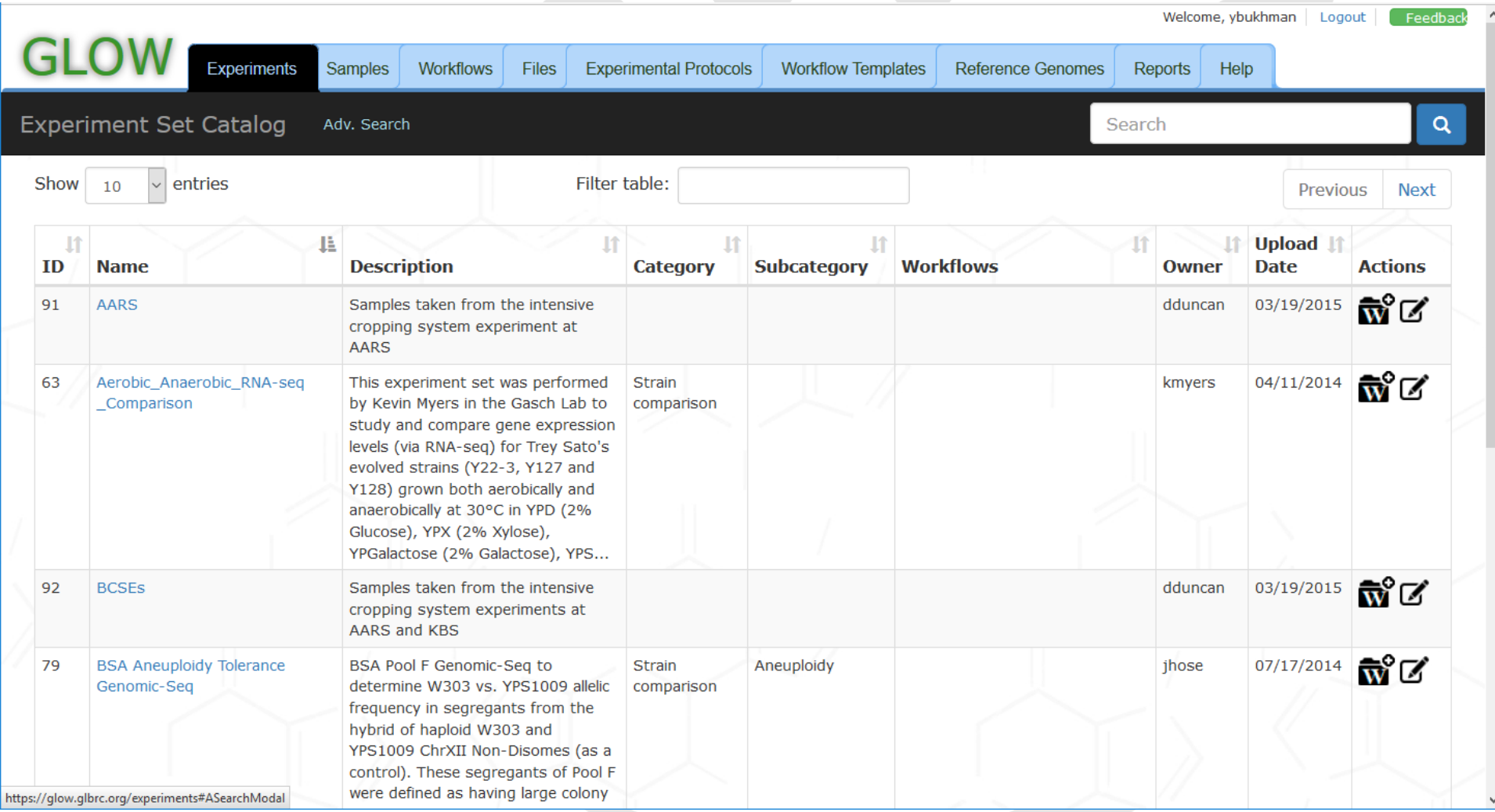
GLOW Experiments



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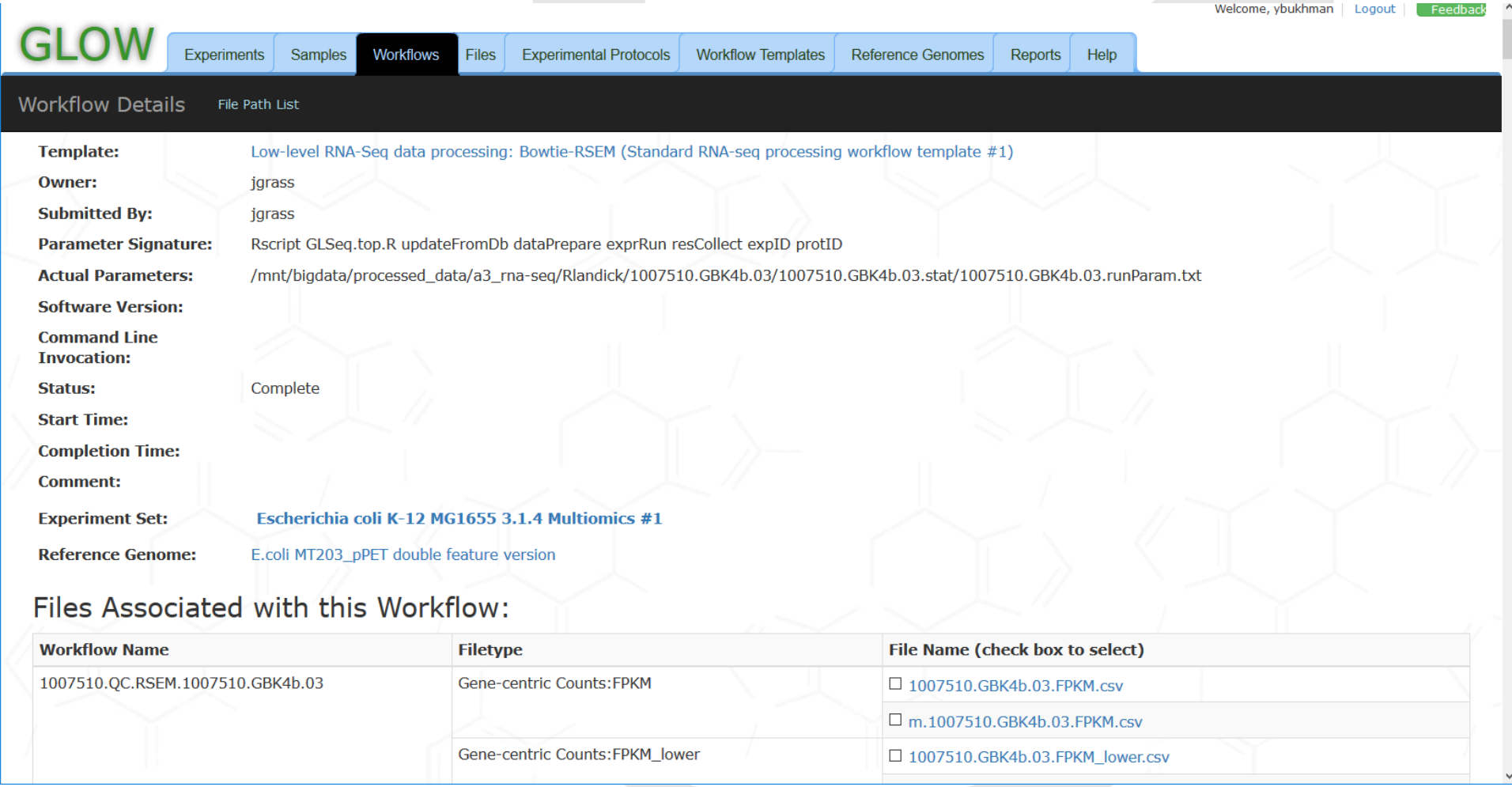
Workflows are Run on Experiment Sets, Consume and Produce Files



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GxSeq Gene Expression Viewer

GLBRC GxSeq

ybukhman | My Account | Log Out

Help | Tools | Samples | Features | Sequence

Expression Viewer - Matrix for: Brachypodium distachyon (Bd21)

Update Selection | Download

Filter Favorites: None

Search definition and locus: Go

(Advanced Options)

← Previous 1 2 3 4 5 6 7 8 9 ... 521 522 Next →

26,091 Matching Results

	Bd_192	tair10	Sbicolor 1.4	CTL-RNAi-pal1-1	CTL-RNAi-pal1-2	RNAi-pal1-1-1	RNAi-pal1-1-2	Sum	Options
| GeneID:100839285 | |				9435.72	6826.8	6553.75	11019.86	33836.13	Details | Graph | Browser
onein-like protein 2C-like	Bradi2g38120.1		Sb05g022840	6039.65	3105.31	2871.86	9070.81	21087.63	Details | Graph | Browser
se small chainPW9,	Bradi3g26391.1	AT1G67090.1	Sb05g003480	4264.48	4556.47	4398.18	3662.85	16881.98	Details | Graph | Browser
se small chainPWS4.3,	Bradi1g65564.1	AT1G67090.1	Sb02g001725	4172.7	4684.72	3873.82	3445.35	16176.59	Details | Graph | Browser
se small chainPWS4.3,	Bradi4g08500.1	AT1G67090.1	Sb02g042765	4193.09	4534.38	3965.85	3044.95	15738.27	Details | Graph | Browser
s; PF03953.7.fs;	Bradi1g10150.1	AT4G14960.2	Sb01g009560	2935.65	3541.07	3257.52	3087.65	12821.89	Details | Graph | Browser
osylmethionine synthase	Bradi2g12160.1	AT4G01850.2	Sb03g013170	2243.15	2260.26	2906.21	2533.62	9943.24	Details | Graph | Browser
842305 |	Bradi1g12787.1	AT4G39260.1	Sb01g012300	2431.77	2192.41	1965.51	2842.94	9432.63	Details | Graph | Browser
; PF00891.8.ls;	Bradi3g16530.1	AT5G54160.1	Sb07g003860	2129.64	1782.27	1959.39	3405.29	9276.59	Details | Graph | Browser
ethyltransferase-like |	Bradi1g13290.1	AT5G17920.2	Sb01g012960	1835.59	2214.82	2885.17	2284.07	9219.65	Details | Graph | Browser
	Bradi4g19457.1	AT4G13940.1	Sb05g014470	1818.18	1888.53	2270.99	2540.1	8517.8	Details | Graph | Browser
02496.6.ls | |	Bradi4g24650.1		Sb08g004190	2084.03	1813.89	1706.95	2717.46	8322.33	Details | Graph | Browser
439.8.ls | |	Bradi2g06220.1	AT3G15353.1		1911.09	2016.92	2088.74	1668.07	7684.82	Details | Graph | Browser
polyubiquitin-like	Bradi3g04737.1	AT5G03240.3	Sb04g004270	2065.79	1757.84	1875.13	1923.75	7622.51	Details | Graph | Browser
ethyltransferase-like |	Bradi4g01200.2	AT3G03780.3	Sb08g022210	1502.49	1755.13	2052.45	1845.14	7155.21	Details | Graph | Browser
LOC100846426 |	Bradi3g01470.1	AT4G35090.1	Sb04g001130	1434.33	1369.15	1790.25	2377.0	6970.73	Details | Graph | Browser
rm 1: chlorophyll a-b	Bradi2g16290.1	AT2G34420.1	Sb03g027030	2201.31	1962.69	1445.91	1066.33	6676.24	Details | Graph | Browser

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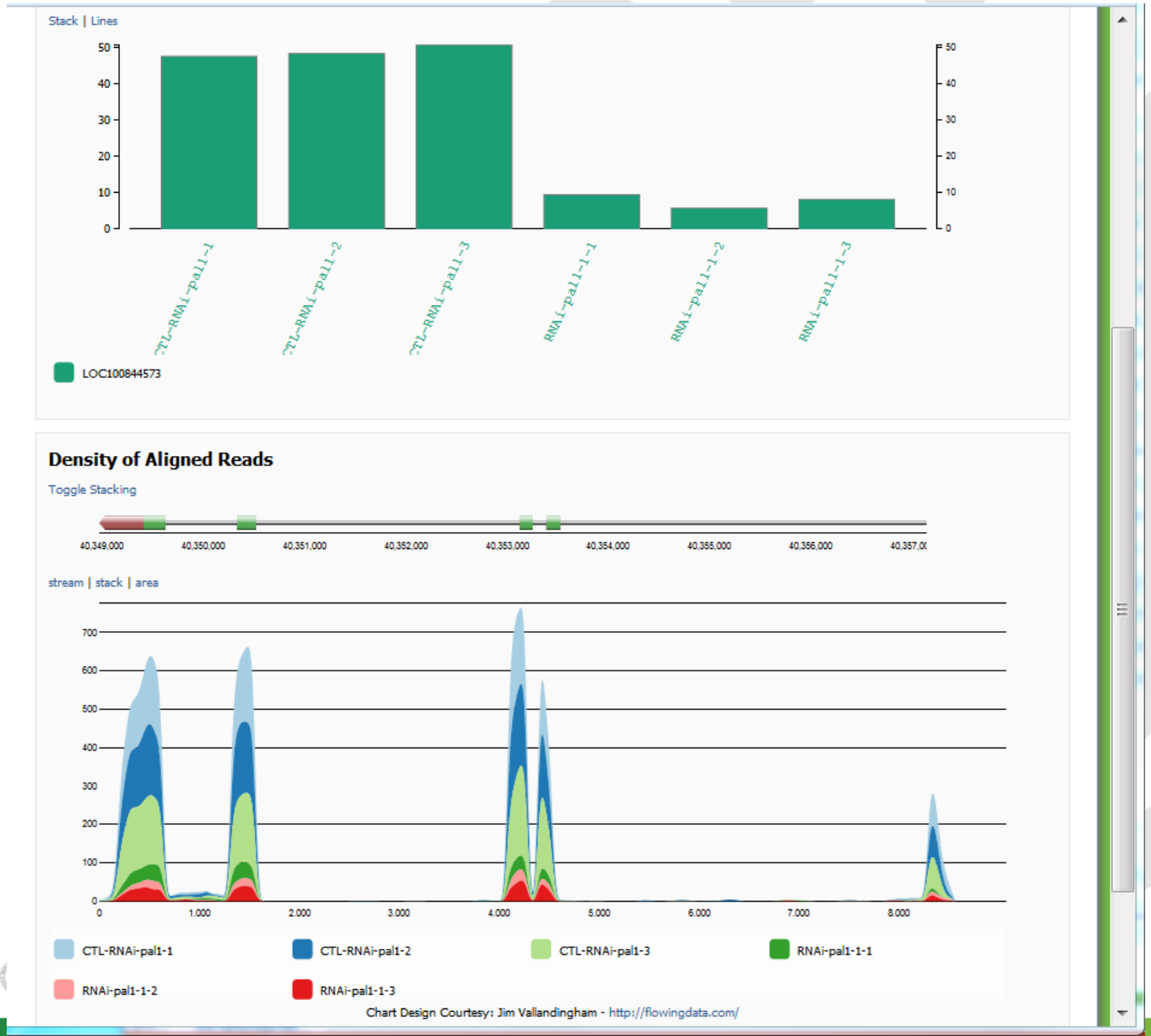
GxSeq Gene View



Nick Thrower,
Matt Larson,
Curt Wilkerson

Open Source

- GxSeq: https://github.com/Michigan-State-University/gxseq (version 1)
- GLOW: coming soon

Acknowledgements

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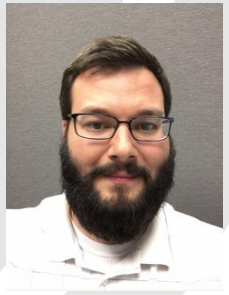
QA/QC: Enhai Xie

GLOW: Darin Kalisak,
Spencer Thiel, Nathan DiPiazza, Adam Halstead, …

Curt Wilkerson, MSU Informatics Group Lead



GxSeq: Nick Thrower,
Matt Larson

THANK YOU

Growing Core Data Management Systems

- Thoughtful design ➔ ability to extend systems and create customized solutions
  - Needs database and software design expertise
  - Needs scientific domain expertise
- Sound software development practices: documentation, version control, testing etc. ➔ maintainable and extensible systems, robust to staff turnover
- Agile: release early, release often ➔ get user input as frequently as possible
- Do well by early adopters ➔ gradually extend reach