



caLIMS v2: cancer
Laboratory
Information
Management
System

A Brief Update for ICR Workspace

August 25, 2010



## Update for caLIMS v2.0



## Today's presentation includes:

- About the development team and community
- Reminder of project description/goals
- Models, method internal workflow, examples, integration plans, and proposed services
- Timeline and development process
- Project Wiki and JIRA Project: sources for additional information about the caLIMS v2 project
- Questions, suggestions, comments, etc.





## Development Team/Community



Collaboration: LPG and CBIIT

- NCI/LPG: Jenny Kelley, Bob Clifford, Cu Nguyen, Henry Zhang
- CBIIT: Anand Basu, Juli Klemm, Robert Shirley, Rachel Shortt
- Moxie Informatics: Sasikumar Thangaraj, Michael Visee, and Mike Connolly
- LS Mentors: Stephen Goldstein, Chris Piepenbring
- SAIC-F: Rod Winkler, Ulli Wagner

caLIMS v2 Development Working Group (DWG): JAX- Abigail
Ames/Grace Stafford, IUPUI – Ganesh Shankar, UT – Scott HunikeSmith, UAZ – Dave Thompson/Nirav Merchant, DFCI – Jomol
Mathew/Erica Jones, UPenn – Avrum Goodblatt, Dartmouth – Paul
Thompson, LabAnswer – Deven Atnoor, UCSF – Mark Bridge/Sudeep
Basnet/Alyssa Lalanne

NCI LIMS Consortium – group interested in LIMS development





The purpose of the caLIMS v2 project is to create a research Laboratory Information Management System (LIMS) that is interoperable within established caBIG® standards and guidelines and will track a complete laboratory workflow that uses materials from a specimen management service (e.g. caTissue) to generate experimental results for one of the caBIG® data management services (e.g. caArray).

## Primary goals for caLIMS v2 include:

- To create an Open Source "near" commercial grade LIMS application that allows laboratories to focus on scientific research and scientific investments.
- To create a general-purpose LIMS application that seamlessly integrates with caBIG® data management systems and analytical tools.
- To develop a generic core LIMS infrastructure that can be used by multiple laboratory types.
- To build a basic LIMS that allows easy extension and customization for a specific Laboratory domain.
- To establish an Open Development Initiative (ODI) that allows LIMS developers to contribute LIMS customizations and enhancements to the end user community.





## caLIMS v2.0 Project Goals



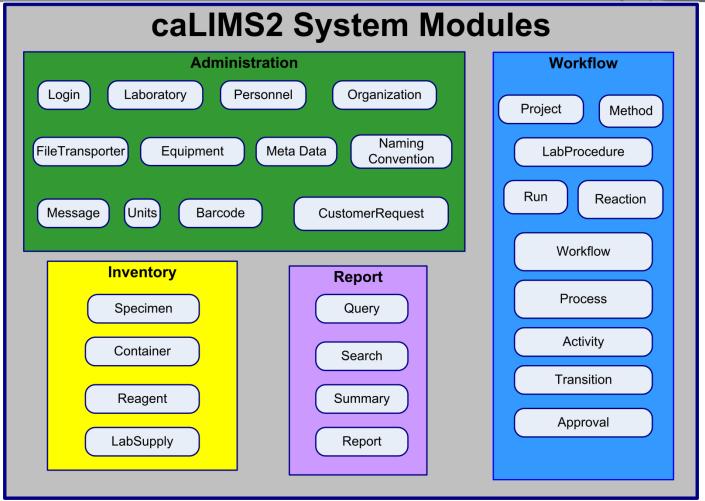
## Functional objectives for the initial implementation of caLIMS v2.0 are:

- to use existing caBIG<sup>®</sup> tools to programmatically search caTissue for specimens with particular characteristics
- to track laboratory activities involving these specimens and all metadata necessary for submitting data files to caArray
- to facilitate the programmatic submission of laboratory data and metadata to caArray
- to record laboratory workflow-specific information such as sample generation and storage conditions, key reagent lot numbers, and parameters for experiments, equipment and software - which may be important for establishing provenance of data submitted to caArray.



## caLIMS v2.0 Core Modules



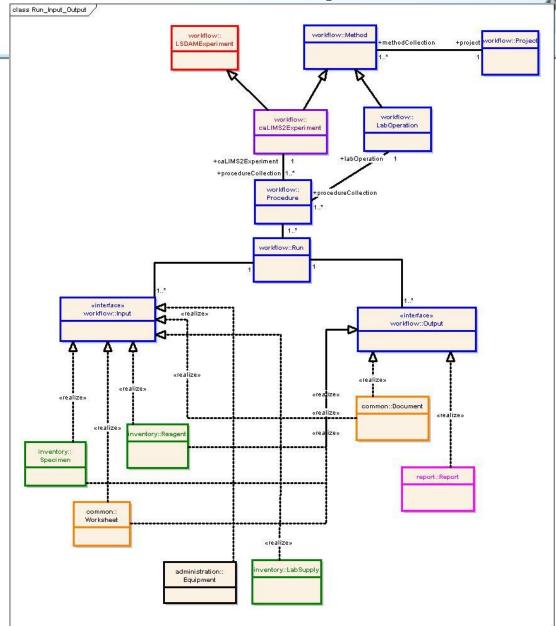


Common classes: Audit, Status, Type, Document, Notes, SOP, EnvironmentalCondition, Events, ExternalIdentifier, Safety, Scheduling.





caLIMS v2.0 OM – Experiment



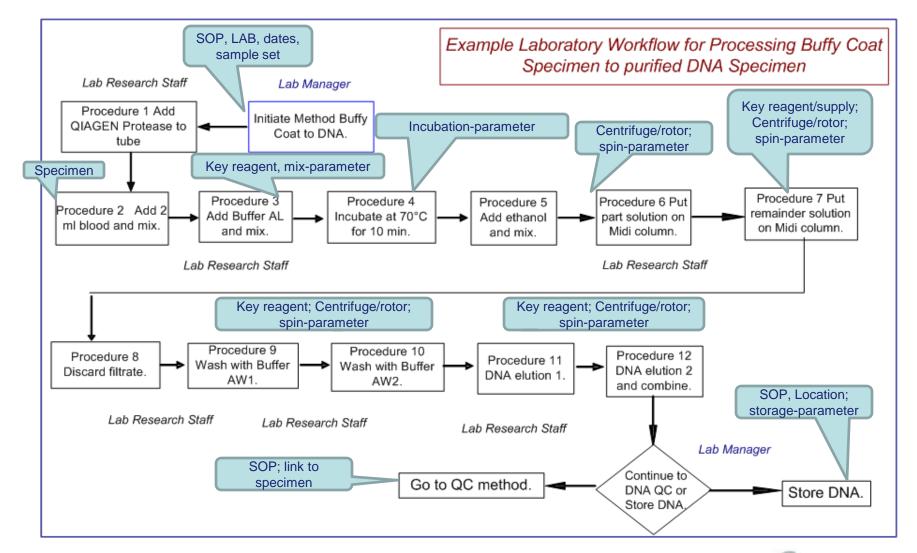






# caLIMS v2.0 Sample Lab Workflow – Specimen processing



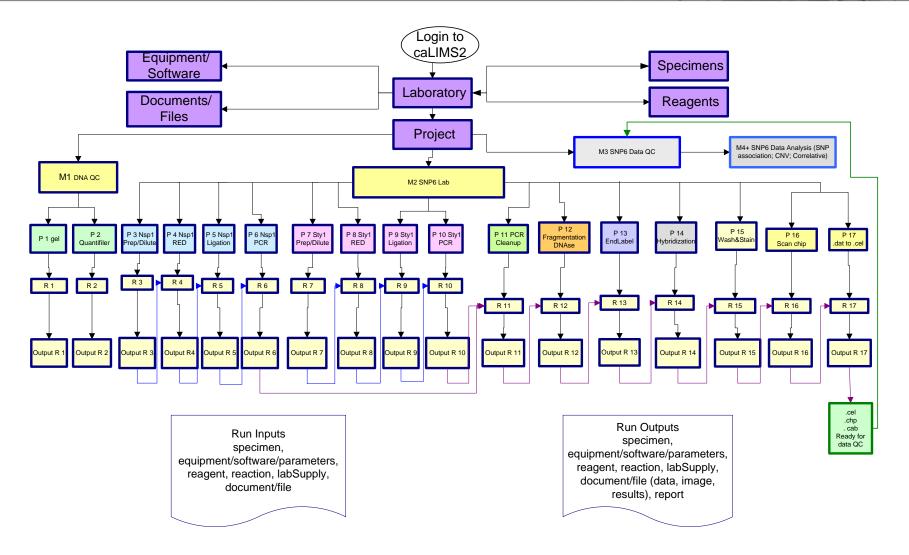






## caLIMS v2.0: Experiment – caLIMS2 Ex. SNP6 wet lab



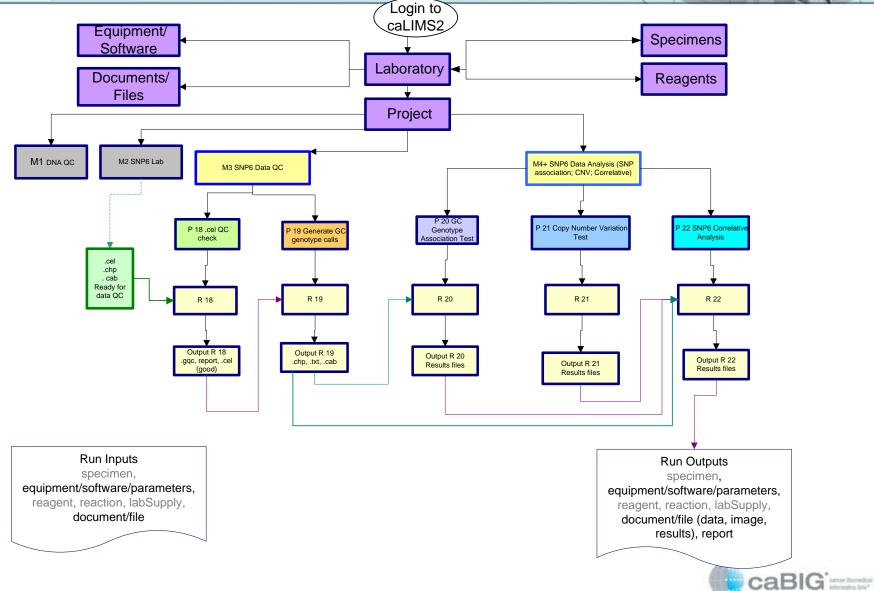






# caLIMS v2.0: Experiment – Ex. SNP6 dry lab



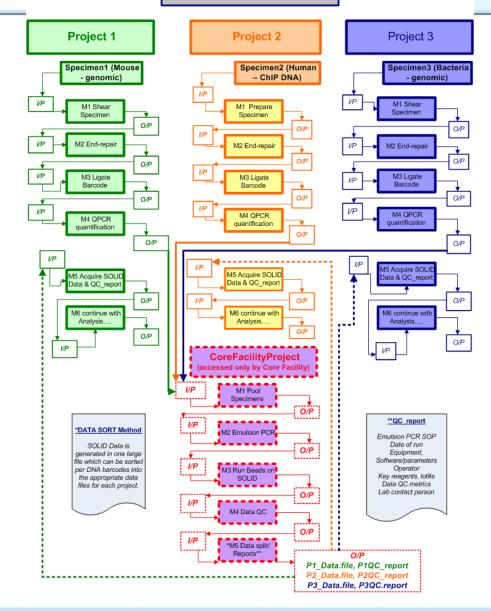




# NexGen Sequencing Workflow



Core Facility Laboratory Workflow







# Proposed Experiment Method Service



caBIG .....

Profile	Operation	Inputs	Outputs	Pre-Conditions
Query	Retrieve an experiment method by: its unique identifier, y experiment attributes (e.g.,name, public identifier, experiment type, method type, equipment type, reagent type, experiment input, experiment output, status), Specimen Type (e.g., Biospecimen, TissueSpecimen, CellSpecimen, NucleicAcid, Protein, etc.), contact/investigator (createdBy, modifiedBy), data type (e.g., gene expression, genotype, or copy number variation), or by any combination of the these criteria with boolean OR/AND	Identifer	List <experiment Method Summary&gt;</experiment 	
Query	Retrieve all details for an experiment method	Identifier	Experiment Method Details: Method (Input, Output, Parameter types, Procedure(s), I/O types, Parameter type, ContactPerson/Org anization)	
Management	Create an experiment method	Experiment Method Details		user authorization
Management	Update an experiment method (e.g.,attributes, Procedures, Equipment Types, Specimen Types, Software Types, Parameters, etc)	Identifier, Experiment Method Details		user authorization
Management	Delete an experiment method	Identifier		user authorization
Management	Update experiment method status	Identifier, Status		user authorization
Management	Import Experiment Method workflow file (as template to create new Experiment Method)	ExperimentMethod File Id		user authorization
Validation	Check if experiment method meets caLIMS2 compliance requirements	ExperimentMethod Id		



## **Proposed Equipment Service**



Operation	Inputs	Outputs	Pre-Conditions
Retrieve an Equipment by: its unique identifier, Equipment attributes (e.g.,name, public identifier, equipment type, propertyID, serialNumber, model, manufacturer, vendor, location, operatingSystem, operatingSoftware, contactPerson, method type, software type, reagent type, Equipment input type, Equipment output type, status), Software Type (e.g., operatingSystem, dataCollection, operatingSoftware, analysisApplication, etc.), contactPerson (investigator) (createdBy, modifiedBy), utput (data) type (e.g., gene expression, genotype, or copy number variation or file type -ab1, .fsa, .cel, .chp, xls, txt, .csv, etc.), input type (e.g., Specimen type, Reagent type, Software type, etc.), or by a combination of the above criteria with boolean OR/AND.	Identifer	List <equipment Summary&gt;</equipment 	
Retrieve all details for an Equipment	Identifier	Equipment Details: I/O types, Parameter type, ContactPerson/Org anization,	
Create an Equipment	Equipment Details		user authorization
Update an Equipment (e.g.,attributes:name, I/O Types, location, Software Types, contactPerson, globalID, propertyID, serialNumber, model, vendor, manufacturer, etc)	Identifier, Equipment Details		user authorization
Delete an Equipment	Identifier		user authorization
Update Equipment status	Identifier, Status		user authorization
Import Equipment template file from an instance of caLIMS2 (as template to create new Equipment service instance from a contributor)	EquipmentFile Id	new Equipment template instance	user authorization
Check if Equipment template instance meets caLIMS2 compliance requirements	Equipment Id	validated Equipment instance	
	Retrieve an Equipment by: its unique identifier, Equipment attributes (e.g.,name, public identifier, equipment type, propertyID, serialNumber, model, manufacturer, vendor, location, operatingSystem, operatingSoftware, contactPerson, method type, software type, reagent type, Equipment input type, Equipment output type, status), Software Type (e.g., operatingSystem, dataCollection, operatingSoftware, analysisApplication, etc.), contactPerson (investigator) (createdBy, modifiedBy), utput (data) type (e.g., gene expression, genotype, or copy number variation or file type -ab1, .fsa, .cel, .chp, xls, txt, .csv, etc.), input type (e.g., Specimen type, Reagent type, Software type, etc.), or by a combination of the above criteria with boolean OR/AND.  Retrieve all details for an Equipment  Update an Equipment (e.g.,attributes:name, I/O Types, location, Software Types, contactPerson, globalID, propertyID, serialNumber, model, vendor, manufacturer, etc)  Delete an Equipment  Update Equipment template file from an instance of caLIMS2 (as template to create new Equipment service instance from a contributor)  Check if Equipment template instance meets caLIMS2	Retrieve an Equipment by: its unique identifier, Equipment attributes (e.g., name, public identifier, equipment type, propertyID, serialNumber, model, manufacturer, vendor, location, operatingSystem, operatingSoftware, contactPerson, method type, software type, reagent type, Equipment input type, Equipment output type, status), Software Type (e.g., operatingSystem, dataCollection, operatingSoftware, analysisApplication, etc.), contactPerson (investigator) (createdBy, modifiedBy), utput (data) type (e.g., gene expression, genotype, or copy number variation or file type -ab1, .fsa, .cel, .chp, xls, txt, .csv, etc.), input type (e.g., Specimen type, Reagent type, Software type, etc.), or by a combination of the above criteria with boolean OR/AND.  Retrieve all details for an Equipment  Update an Equipment (e.g., attributes:name, I/O Types, location, Software Types, contactPerson, globallD, propertyID, serialNumber, model, vendor, manufacturer, etc)  Delete an Equipment  Update Equipment status  Import Equipment template file from an instance of caLIMS2  (as template to create new Equipment service instance from a contributor)  Check if Equipment template instance meets caLIMS2  Equipment Id	Retrieve an Equipment by: its unique identifier, Equipment attributes (e.g., name, public identifier, equipment type, propertylD, serialNumber, model, manufacturer, vendor, location, operatingSystem, operatingSoftware, contactPerson, method type, software type, reagent type, Equipment input type, Equipment output type, status), Software Type (e.g., operatingSystem, dataCollection, operatingSoftware, analysisApplication, etc.), contactPerson (investigator) (createdBy, modifiedBy), utput (data) type (e.g., gene expression, genotype, or copy number variation or file type -ab1, .fsa, .cel, .chp, xls, txt, .csv, etc.), input type (e.g., Specimen type, Reagent type, Software type, etc.), or by a combination of the above criteria with boolean OR/AND.  Retrieve all details for an Equipment  Update an Equipment (e.g., attributes:name, I/O Types, location, Software Types, contactPerson, globalID, propertyID, serialNumber, model, vendor, manufacturer, etc)  Delete an Equipment  Update Equipment  Update Equipment template file from an instance of caLIMS2 (as template to create new Equipment service instance from a contributor)  Check if Equipment template instance meets caLIMS2  Equipment Id  Validated





# caLIMS v2.0: timeline – rough estimate



- Use case model completed
- Logical model completed and submitted to caDSR
- caLIMS v2.0.0.5M1 (sample inventory search only) released
- caLIMS v2.0
  - Funding for FY2010: 1 lead architect + 2 full time resources
  - Q1 completion of v1.0 OM and submission to caDSRdone
  - Q2 Construction began (Infrastructure + Administration module (Aug. 24, 2010)
  - Q3 Inventory and Report module
  - Q4 Workflow module
  - 2011 Q1/Q2 release caLIMS v2.0 with features in scope and basic workflow plus report functionalities (caLIMS v2.0 DWG members/early adopters)





## caLIMS v2.0: timeline - dates



TASK	DAYS	FROM	ТО
Inception + elaboration	45	3/25/2010	5/24/2010
Construction I	52	5/25/2010	8/5/2010
Transition 1	11	8/6/2010	8/20/2010
Construction II	60	8/23/2010	11/16/2010
Transition 2	10	11/17/2010	12/2/2010
Construction III	47	12/3/2010	2/8/2010
Transition 3	29	2/9/2011	3/23/2011





## caLIMS v2 Project: NCI JIRA



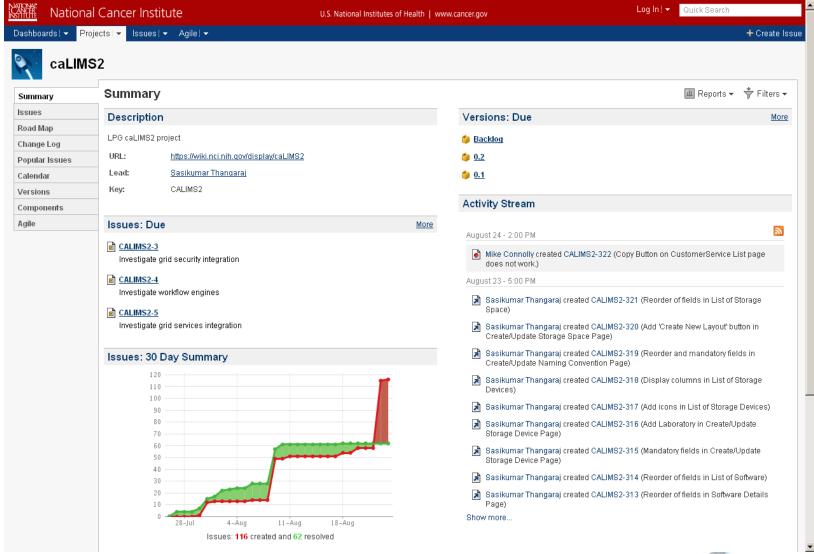
National Cancer Institute	U.S. National Institutes of Health   www.cancer.gov	+ Creat
duction	Login	
***WARNING**  are accessing a U.S. Government information system, which puter network, (3) all computers connected to this network, a ched to this network or to a computer on this network. This int ernment-authorized use only. Unauthorized or improper use on on, as well as civil and criminal penalties.  sing this information system, you understand and consent to outhave no reasonable expectation of privacy regarding any ce ed on this information system. At any time, and for any lawful monitor, intercept, and search and seize any communication mation system.  ny communication or data transiting or stored on this informa iny lawful Government purpose.  To create a new account in JIRA, plea Create Account	includes (1) this computer, (2) this d(4) all devices and storage media formation system is provided for U.S. of this system may result in disciplinary the following:  communications or data transiting or 30 overnment purpose, the government or data transiting or stored on this tion system may be disclosed or used	a member? Contact an Administrator to request an account.  Log In
ects		
2B (CAB2B)  Baris Suzek	<u> </u>	
id Services Security (CSS)  Braulio Cabral	<u> </u>	
<b>1S2</b> (CALIMS2) Sasikumar Thangaraj	ш → 👸 →	
OD (CAMOD) Ulrike Wagner	ш - 🐈 -	
BDA (BDA) Steven Saksa	<u> </u>	
	- +	





## caLIMS v2 Project: NCI JIRA









## caLIMS v2 Project Wiki



🕮 Tools 🔻



## · caLIMS2 Wiki Home page

by Ann Wiley, last edited by Sasikumar Thangaraj on Aug 23, 2010 (view change)

#### ents

- Overview of caLIMS2
- Using the caLIMS2 Wiki

#### ware

- caLIMS2 Software
- caLIMS2 Development
- caLIMS2 Download
- caLIMS2 GForge project
- Report Bugs

#### Content

- caLIMS2 Wiki Home
- caLIMS2 Background
- caLIMS2 Project Goals
- caLIMS2 Overview
- caLIMS2 Features
- caLIMS2 Documentation
- caLIMS2 Collaborations
- caLIMS2 Presentations
- caLIMS2 Development Working Group
- caLIMS2 Software
- caLIMS2 Communication
- NCI LIMS Consortium
- caLIMS2 Community Input
- caLIMS2 Deployment Artifacts
- caLIMS2 Contact Us

### Overview of caLIMS2

The purpose of the caLIMS2 project is to create a Laboratory Information Management System (LIMS) that is interoperable within established caBIG® standards and guidelines and will track a complete laboratory workflow that uses materials from a specimen management service (e.g. caTissue) to generate experimental results for one of the caBIG® data management services (e.g. caArray). Core LIMS functions include the management of personnel, equipment, lab supplies and reagents, samples, laboratory workflow and experimentally derived metadata and data, caLIMS2 will complete the caBIG® bench to bed model by bridging the gap between biospecimen repositories, data repositories and analysis tools. The application is designed to allow easy customization by users and to facilitate integration with laboratory equipment, analytical tools and data sources, caLIMS2 is highly flexible, making it suitable for use by research labs, high throughput core facilities and public health labs, caLIMS2 will help further translational cancer research through the organization of laboratory workflow, tracking of specimens, acquisition of laboratory data and metadata, and the appropriate sharing and dissemination of the data to support subsequent analyses. More information and project details can be found using the following links. If you have guestions, please contact Robert Clifford or Jenny Kelley,

- caLIMS2 Project Goals
- Project Background
- Project Overview
- Product Features
- Project Documentation
- Project Collaborations
- caLIMS2 Presentations
- caLIMS2 Software and Development
- caLIMS2 Development Working Group
- caLIMS2 Communication
- caLIMS2 Community Input
- caLIMS2 Deployment Artifacts
- caLIMS2 Contact Us

### Using the caLIMS2 Wiki

This is the wiki home page of calIMS2 (Cancer Laboratory Information Management System 2). Project team members may edit this page and add more pages. Any user may add a comment and we welcome feedback!





## caLIMS v2 Project Wiki





National Cancer Institute



New Account Helpful Tip

<u>Dashboard > ICR - caLIMS2 > caLIMS2 Wiki Home page ></u> caLIMS2 Development Working Group

Browse ▼ Log In



## acaLIMS2 Development Working Group

tis Tools ▼

Added by Jenny Kelley, last edited by Jenny Kelley on Aug 17, 2010 (view change)

#### Contents

- · caLIMS2 Development Working Group Overview
  - Meeting
  - Information
  - · Community Input Special Interest
  - Working Groups (SIGs)
  - · Design artifacts and detailed documentation
- caLIMS2 Development Group Members:

### caLIMS2 Development Working Group Overview

The goal of the caLIMS2 project working group is to provide input and guidance to the development of an open source Laboratory Information Management System (LIMS) that is caBIG® silver compliant and will be easy to customize and extend to support multiple disciplines (genomics, proteomics, etc.) and laboratory types basic research, clinical research, public health, and core facilities. Communities interested in having input to the design and development of the application or who have an interest in being an early adopter are welcome to join!

To join the working group, send email request with full name, affiliation, and email address to Jenny Kelley or to Bob Clifford).

### Meeting Information

There are regular working group meetings on the first and third Tuesdays of the month at 1 pm Eastern time. Communication is through these meetings and meeting notes, this wiki, and the NCI LIMS Consortium List-serve. We anticipate having a community Forum site set up within this Wiki site sometime in the near future. Development meeting notes can be found on our GForge site using this link: caLIMS2 DWG meeting notes. If you would like more information or would like to join the DWG, please contact Jenny Kelley or Bob Clifford,

#### Wiki Content

- caLIMS2 Background
- caLIMS2 Project Goals
- caLIMS2 Overview
- caLIMS2 Features
- caLIMS2 Documentation
- · caLIMS2 Collaborations
- caLIMS2 Presentations
- · caLIMS2 Development Working Group
- caLIMS2 Software
- caLIMS2 Communication
- NCI LIMS Consortium
- · caLIMS2 Community Input
- caLIMS2 Contact Us

Community Input

For additional ways to contribute input to the caLIMS2 Development team, please see the: caLIMS2 Community Input page. We are now gathering laboratory workflow examples from our community which will guide the development team as they create template laboratory workflows for the caLIMS2.

### Special Interest Working Groups (SIGs)

More information on the caLIMS2 SIGs can be found on the SIG pages:

Interface SIG (ISIG)

Business Information Management, Object Model, Analysis, Barcode & RF SIGS

### Design artifacts and detailed documentation

Design artifacts and detailed information can be found on the Documentation page.

### caLIMS2 Development Group Members:

Project/Affiliation Name



## caLIMS v2.x Iteration 1 Welcome



National Cancer Institute	U.S. National Institutes of Health   www.cancer.gov
caLIMS2	Laboratory of Population Genetics
Welcome to caLIMS	⊕ Help



caLIMS2 version 1.0 will be an open source basic Laboratory Information Management System which will support programmatic integration with caBIG® applications and services - for example caArray and caTissue. The caLIMS2 core application will provide the functions needed for basic research laboratory operations. These include functions for managing users and groups, equipment, key reagents and supplies, specimens and their derivatives, laboratory workflow, experimental results, quality control, and reports An internal adaptive workflow engine will enable users to easily create new and/or modify existing laboratory 'template' workflows to fit the specific needs of their laboratories; in addition, these workflow templates can be shared with other caLIMS2 instances. The core caLIMS2 v1.0 application will support the generic molecular biology domain; however, the flexible design will enable later releases of caLIMS2 to be customized for additional specific domains, such as next generation sequencing, nanoparticle characterizations, model organism research, or proteomics, by the integration with existing caBIG® applications or the addition of new modules.

### Features

#### Administration Module

- Create Organizations/Laboratories
- ▶ Create Persons/Contact Information/Roles
- ▶ Create Collaborations
- ▶ Create Equipment/Software
- ▶ Create Locations/Storage Space
- ▶ Create Customer Accounts
- ▶ Create Naming Conventions

### Latest News

Work on CII I1 will begin end of August.

Construction 1 phase completes August 20.

Follow caLIMS2 development progress on the caLIMS2 wiki.

Interested parties are invited to join the caLIMS2 Development Working Group.

The caLIMS2 development team welcome submission of laboratory experiment workflows.

DWG meeting notes and presentations are available.

CONTACT US

PRIVACY NOTIC

MED

ITY APPLICATION













# caLIMS v2.x I1: SU access to all





Today is: 8/25/10

Welcome: Super User

Your Current Projects:

Laboratory Updates:

CONTACT US

PRIVACY NOTICE

D1001 01145

BILITY APPLICATION SI





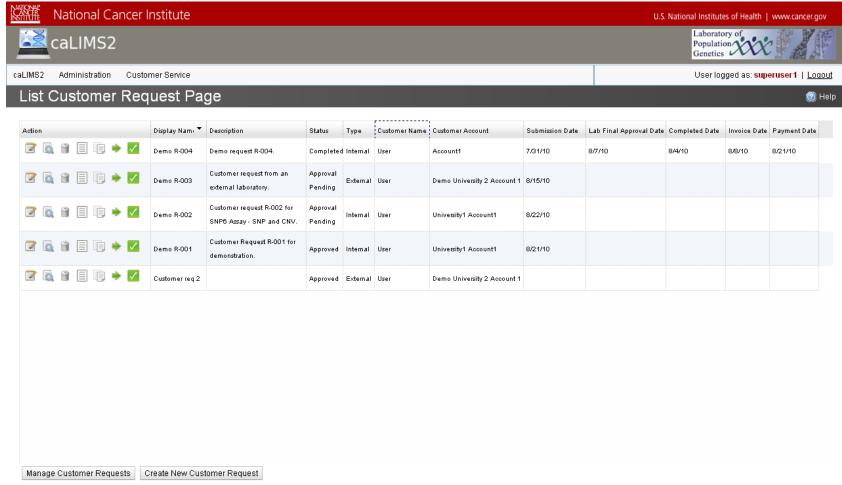






# caLIMS v2.x I1 security SU1/CR





CONTACT US

PRIMACY MOTH

/ APPLICATION S







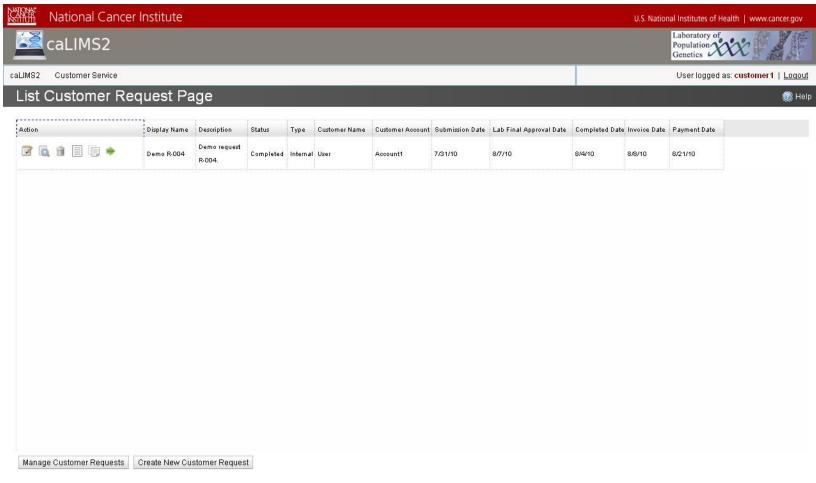






# caLIMS v2.x I1- security C1/CR

















# caLIMS v2.x I1 LabManager- Org





Action	Display Name	Description	Status	Туре	DUNS Number	ldentifier Number	Is Tax Exempt?	Legal Category Type	Location	Parent Organization
	CCR	More than 250 scientists and clinicians working in intramural research at NCI.	Active	Federal Government			true	Federal Government	Bldg. 10	NCI
	Demo University2	Another University for demonstration.	Active	University	343343343		false	Education	Demo University 2 Location 1	
	Demo University1	A University for demonstration purposes.	Active	University	131131131	242242424	false	Education	Demo University1 Location1	
	LPG	A Laboratory in the NCI/CCR that utilizes genetic analysis to gain insight into biologic processes.	Active	Federal Government			true	Federal Government	NIH Bidg. 41	CCR
	NCI	NCI leads a national effort to eliminate the suffering and death due to cancer.	Active	Federal Government			true	Federal Government	Bldg. 10	NIH
		NIH - seek fundamental knowledge about nature & behavior of living systems; reduce burden of disease							NIH-Bethesda	
	Test Organization1	Demo test organization1	Active	Test Organization Type	111111111	demo1idnumber	true	Federal Government	Bldg. 10	NIH
	Test Org2		Active	Institution					EJ2115	Test Organization1

Manage Organizations

Create New Organization

CONTACT US PRIVACY NOTICE DISCLAIMER ACCESSIBILITY APPLICATION SUPPORT





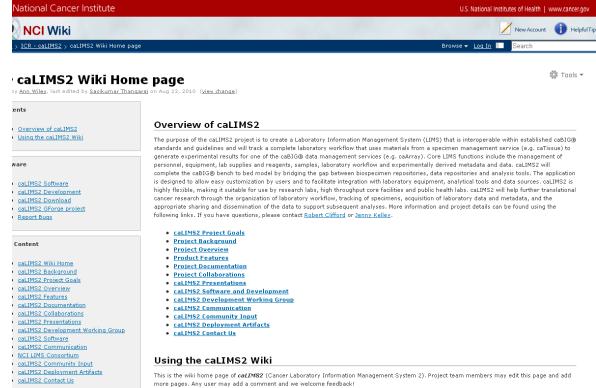






## caLIMS v2 - communication





### caLIMS v2 Project Wiki:

https://wiki.nci.nih.gov/x/2oMYAQ

### caLIMS v2 NCI GForge site:

http://gforge.nci.nih.gov/projects/calims2

caLIMS v2 JIRA: https://tracker.nci.nih.gov

### **Contacts:**

Jenny Kelley<sup>1</sup>: <u>kelleyj@mail.nih.gov</u>

Bob Clifford<sup>1</sup>: clifforr@mail.nih.gov

Sashi Thangaraj<sup>2</sup>: <a href="mailto:sashi@moxieinformatics.com">sashi@moxieinformatics.com</a>

1) NCI Laboratory of Population Genetics, 2) Moxie Informatics





## caLIMS v2: Update end



• Questions, suggestions, comments, etc.

