QTreds: a flexible LIMS for omics laboratories

NETTAB 2012
16th November, 2012

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 CRS4

- CRS4 founded in 1990 by C. Rubbia and P. Zanella
- Sardinian Technology Park

- Focus Areas:
  - Data Fusion
  - Information Society (ICT)
  - Energy and Environment
  - Biomedicine
Overview

✦ Introduction
✦ Motivation
✦ Core Modules
✦ Conclusions
✦ Future perspectives
Motivation

✧ High-throughput technologies and data explosion
✧ The development of complex lab procedures
✧ A LIMS to efficiently handle these issues
✧ What is a Lims?
QTreds and CGSP

What is it

QTreds is a LIMS
What is it

QTreds is a LIMS
QTreds for:

- Tracking and monitoring lab activities
- Quality control and error tracking
- Access control policy
- Sample handling
Our approach

An anthropological approach

Bronislaw Malinowsky

“to grasp the native’s point of view, his relation to life, to realize his vision of his world”

(Argonauts of the Western Pacific, 1961)
<table>
<thead>
<tr>
<th>Sample name</th>
<th>Project</th>
<th>Sample type</th>
<th>Organism</th>
<th>Investigator</th>
<th>Lab</th>
<th>Concentration</th>
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<td>rRNA</td>
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Related issues

- Data Sharing
- Scalability
- Access Control
- Data Integrity Loss
- Data Redundancy
Dealing with complexity
Managing complex protocols

DNA Library Preparation

Exome Enrichment
From this
From this
to this
QTreds overview
MVC divides the work of the application into three separate but closely cooperative subsystems.
Development tools

- Web-based application
- The Ruby programming language
- The Rails framework

Wednesday, 21 November 2012
QTrad functional blocks

- Workflow Generator
- Sample Handler
- Inventory Management System
- User Management System
Key point: Protocol definition
Protocol: the sequence of steps of an experiment
Each experimental protocol is defined as XML document

XSD to define:
- structure
- elements
- attributes
- constraints
Long and boring task

List of:
- activities
- instruments
- reagents
- items ...
Visual Tool

### Visual Tool for LIMS 0.1 Beta ###

** THIS IS THE WORKBENCH **

[x] Activity element1_activity

[x] Input element2_input

[x] Label element1_label

---

X=958 Y=471

activity  instrument
input  close
attribute  label
Sample handling

- **Qtreds** records:
  - the path of each sample – chain of custody

- **Storage Location Management**

- allows to handle:
  - One sample at a time
  - Multiple samples

- Multiple samples can be combined into one entity (**Pooling**)
Inventory Management

- Reagents, lab glassware and consumables easily added through their **barcodes**

- **Minimum stock levels** can be handled to avoid shortages of essential products
Catalog where all categories of items have to be inserted
Stock to register all consumables in the lab
Topology a virtual representation of the lab to keep track of the locations
Personal Stock a sort of “shopping cart”
Centralized Authorization Function

User | Request | Role

\[ F(U, R, R[]) \]
Multiple roles
Multiple roles

✧ Admin
✧ Supervisor
✧ Inventory manager
✧ User
✧ Analyzer
Multiple roles

- Admin
- Supervisor
- Inventory manager
- User
- Analyzer

A user can have different roles
Multiple roles

- Admin
- Supervisor
- Inventory manager
- User
- Analyzer

A user can have different roles

F(U, R, R[])
Other features

- **Internal Messaging System** a collaborative tool to allow users to interact with each other
- **REST API** to allow an automated access to information
QTreds and the **CRS4 Sequencing and Genotyping Platform (CSGP)**

Different kinds of experiments:

- DNA Library Preparation
- Exome Enrichment
- Sequencing
Collaborations

Chemistry

Proteomics

Genomics

Genetics

Virology

Metabolomics
Future perspectives

✧ New version early 2013
✧ New features:
  – Plugin system to directly interface instruments to QTreds
  – Ad-hoc reporting visual tool to create your own reports
  – ”Calendarization” system to schedule the activities and the workload balancing
# DS3 group

<table>
<thead>
<tr>
<th>Personnel</th>
<th>Expertise</th>
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</thead>
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<tr>
<td>Patricia Rodriguez-Tomé</td>
<td>Bioinformatics, Seismology (HEAD)</td>
</tr>
<tr>
<td>Giuliana Brunetti</td>
<td>Biology, Science dissemination</td>
</tr>
<tr>
<td>Gianfranco Frau</td>
<td>Computer Engineering</td>
</tr>
<tr>
<td>Elisabetta Marras</td>
<td>Statistics</td>
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<tr>
<td>Piergiorgio Palla</td>
<td>Computer Engineering</td>
</tr>
<tr>
<td>Luana Vargiu</td>
<td>Biology</td>
</tr>
</tbody>
</table>
The End
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Thanks for your attention!
The End

Thanks for your attention!

http://qtreds.crs4.it/demo
user: labuser
psswd: qtreds