

Laboratory Information Management Systems

- **Computerized systems to track, manage, and facilitate processing of samples and data and integrate data analysis**
- **Pre-LIMS**
 - Notebooks, spreadsheets, files, folders...
 - Experimental data in various, incompatible formats
 - Data analysis limited to single experiments
 - Access privileges difficult to enforce

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Typical LIMS Features

- **Logistics management**
 - Data storage and maintenance
 - Inventory tracking
 - Ownership audit trails
- **Designed for laboratory use**
 - Barcode tracking of samples
 - Workflow tracking (SOP)
 - Interface to instrumentation for data collection/import
- **Integrated Data Analysis tools**

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ActivX Biosciences, Inc.

- **Drug discovery & development company**
- **Unique protein activity analysis technology**
- **Founded in April of 2000**
- **Currently 40 employees**
- **Internal drug development program with focus on oncology**
- **Collaborations with pharmaceutical industry**

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The logo for ActivX Biosciences, Inc. features the word "ACTIV" in a bold, sans-serif font. To the right of the text is a stylized graphic consisting of a white and grey 'X' shape with a small black dot at its center, set against a blue background.

LIMS Requirements at ActivX

- **Versatility**
 - Three major technology platform components
 - Several types of data
 - Need to integrate with commercial and public database contents
- **Scalability**
 - Initial storage requirements expected to grow greatly in the future
- **Maintainability**

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Specific Needs - Data Storage

- **Proteomics data**
 - Protein identification by mass spectroscopy
 - Quantification by gel & capillary electrophoresis and mass spec
- **Medicinal chemistry data**
 - Commercial chemical compound database
 - Activity data for candidate drug molecules
 - Inventory of chemicals
- **Biological Sample data**
 - Tracking & categorization of samples
 - Treatment information

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Specific Needs - User Access

- **Simple and intuitive user interfaces**
- **Web based access**
 - Platform independence
 - Maintainability with fewer resources
- **Project based access privileges**
- **User authentication**
- **Data & analysis result export**

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Specific Needs - Analysis

- **Cross-platform integration**
 - Data capture from various instruments
- **Cross-experiment integration**
 - Data capture from commercial software packages
- **Backend high-performance access for CPU/memory intensive analysis**

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Commercial LIMS Systems

- **Many vendors**
 - <http://www.limsources.com/>
- **No complete “off-the-shelf” product**
- **Very few open-source products**
 - Essential for in-house adaptation & maintenance
- **High license and support costs**

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Open-Source, GPL LIMS

- **General**
 - WIFlow - Generic workflow, pre-alpha
 - Gnosis(the LIMS) - python/C, planning stage
 - FreeLIMS - coming soon
- **Application Specific**
 - HalX - Structural Genomics, alpha
 - AMAD, ArrayDB, BASE... - Microarray

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ActivX In-House Solution

- **Use of mature, open-source & free components**
- **Tiered system architecture**
- **Relational database backend**
- **Data model driven business layer**
- **Template & MVC based front end**

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Tiered Framework Architecture



Template engine
Java-based MVC implementations



Servlet framework
secure, web application layer



Persistence layer
peer based Object relation model



Relational database
storage system

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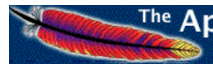
Open-Source Throughout



The **Apache Jakarta Project**

<http://jakarta.apache.org/>

-> Turbine & Velocity



The **Apache DB Project**

<http://db.apache.org/>

-> Torque



<http://www.mysql.com>



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Data and Software Integration

- **Data import**
 - Legacy data
 - Commercial software output
 - NT Domain authentication
- **Data Analysis tools**
 - MatLab
 - gnuplot
 - R package
 - PtPlot/JFreeGraph

Open-Source!

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Open-Source Advantages

- **Massive influx of ideas & contributions**
- **Flexibility**
- **No “surprises”**
- **Reliability**
- **Able to modify it as needed**
- **“Push it forward” mentality of community**
- **Large support base for popular packages**
- **IP of open-source based system with developer**

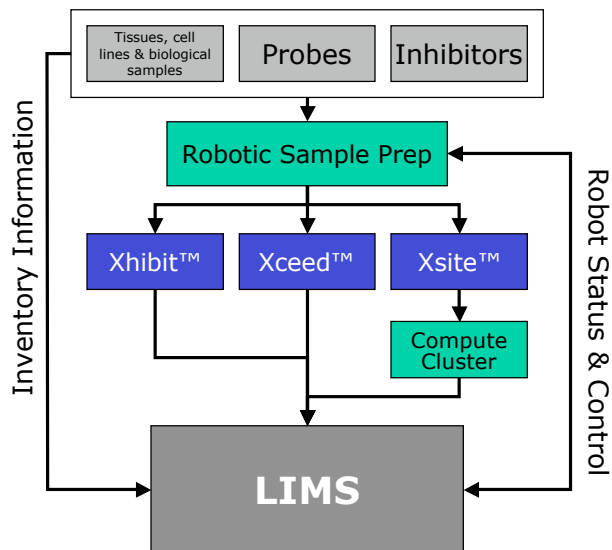
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Open-Source Disadvantages

- Support not guaranteed
- Unpredictable development cycles
- (FDA validation requirements)

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Information Flow Overview



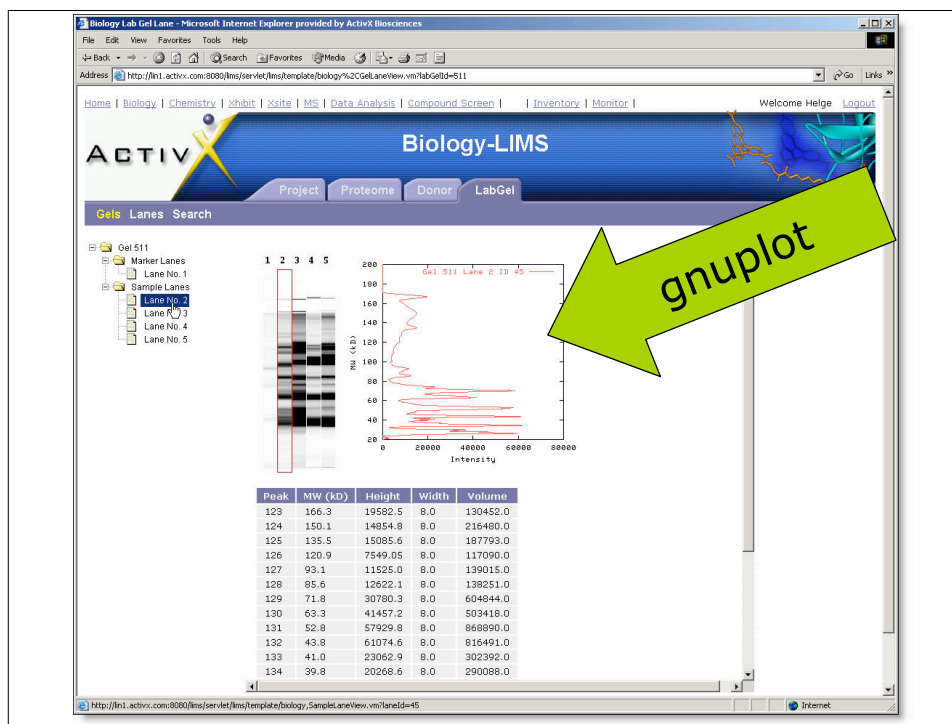
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Conceptual LIMS Sections

- Chemistry
- Biology
- Xhibit™ - High-throughput gel electrophoresis
- Xsite™ - MS based peptide ID & quantification
- Xceed™ - High-throughput capillary electrophoresis
- Data Analysis
- Compound Screen
- Inventory

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The screenshot shows a web browser window titled "Bioinformatics - Microsoft Internet Explorer provided by ActivX Biosciences". The address bar shows "http://bioinformatics.activ.com/". The website header features the "ACTIV" logo and the word "Bioinformatics". Below the header is a "Welcome Hodge" message. The main content area is titled "ActivX Data Systems" and contains a grid of icons and links for various systems: XHIBIT LIMS, XSITE LIMS, MS LIMS, Clinical Samples, Cell Line Samples, Animal Samples, Small Molecule, Probe, Proteome, Data Query & Analysis, Databases & Tools, and SOP Documents. To the right, there are sections for "News", "Journals", and "References", each with a list of links. At the bottom, there are sections for "Public Databases", "DNA Analysis", "Genome Centers", "Discussion Board", "Protein Analysis", "Current Sequencing Projects", "Biological Resources & Information", and "Bioinformatics Report".



The screenshot shows the Chemistry-LIMS web interface. The main area displays an inventory table with columns for Barcode, Chemical, Amount, Location, and Date Received. An 'Edit Inventory' dialog box is open, showing fields for Name, Barcode, Cas #, Catalog, Amount, and Location, along with a 'Save Changes' button.

Barcode	Chemical	Amount	Location	Date Received
19885	diisoamylamine			Feb 3, 2004
19884	3-(butylamino)propanol			Feb 3, 2004
19883	lithium azide			Feb 3, 2004
19882	cyclopentanone			Feb 3, 2004
19881	1-bromo-4-methylpent			Feb 3, 2004
19880	2-hexanone			Feb 3, 2004
19879	protriptyline hydrochlor			Feb 3, 2004
19878	2,6,6-trimethyl-1-cyclohex			Feb 3, 2004
19877	1-acetaldehyde			Feb 3, 2004
19877	maprotiline hydrochlor			Feb 3, 2004
19876	1-adamantaneethane			Feb 3, 2004
19875	2-cyclohexylethyl bromide	1 gram	11025/120 hood 2	Feb 3, 2004
19874	4-tert-butylcyclohexanone	25 gram	11025/120 hood 2	Feb 3, 2004
19873	4-nitrobenzoic acid	250 gram	11011 hood 5	Feb 3, 2004
19872	4-nitrobenzoyl chloride	50 gram	11011 hood 5	Feb 3, 2004
19871	tert-butylamine	100 mL	11011 hood 5	Feb 3, 2004
19870	boc-6-aminohexanoic acid-osu	1 gram	11011 hood 4	Feb 3, 2004
19869	boc-6-aminohexanoic acid-osu	1 gram	11011 hood 5	Feb 3, 2004
19868	n-isobutyl-o-t-butylxyethyl amine	1 gram	11025/120 hood 2	Feb 3, 2004
19867	n-isopropyl-o-t-butylxyethyl amine	1 gram	11025/120 hood 2	Feb 3, 2004
19866	acetonitrile	4 Liter	11025/130 MS lab	Feb 2, 2004

Home | Biology | Chemistry | Xhibit | Xsite | MS | Data Analysis | Compound Screen | Inventory | Monitor | Welcome Helge Logout

ACTIV X Chemistry-LIMS

Inventory

Receiving Listing Discard **Search** History

Substructure Search

Search Inventory! Search ACD

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The screenshot shows the Chemistry-LIMS interface. At the top, there is a navigation bar with links to Home, Biology, Chemistry, Xhibit, Xsite, MS, Data Analysis, Compound Screen, Inventory, and Monitor. The main header features the 'ACTIV X' logo and 'Chemistry-LIMS'. Below this, there is a sub-header for 'Inventory' with tabs for Receiving, Listing, Discard, Search, and History. The 'Search' tab is active. A 'Substructure Search' window is open, displaying a periodic table of elements. The element 'Au' (Gold) is highlighted, and its properties are shown: Mass: 196.9665, Density: 19.3, Oxidation States: +1, +3, and Electron Configuration: -32-18-1. The search window also includes a search bar and buttons for 'Search Inventory!' and 'Search ACD'. At the bottom, there is a copyright notice: 'Powered by the ActivX Bionformatics Team Copyright © 2002-2003 by ActivX, Inc'.

Home | Biology | Chemistry | Xhibit | Xsite | MS | Data Analysis | Compound Screen | Inventory | Monitor | Welcome Helge Logout

ACTIV X Inventory-LIMS

Proteome Probe Smolecule MolMarker Chembio

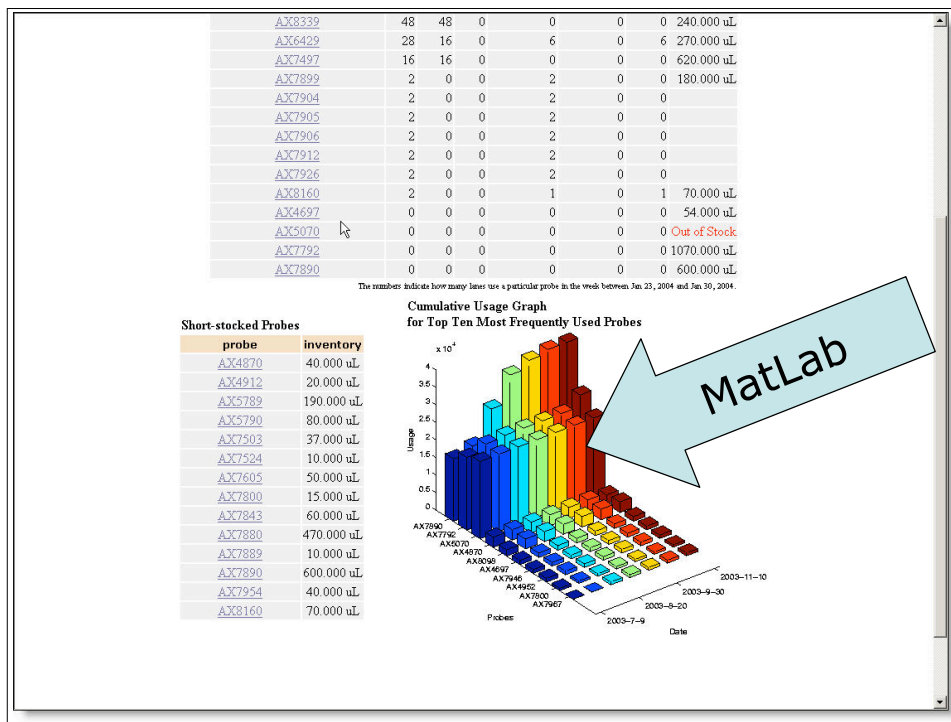
InventoryAdd InventoryView

Add Total 30 Pages Search

Inventory	Probe	Axnumber	Name	Alias	Formula	Structure	EntryIs
	61	AX4609			C13 H22 N2		206.331 1042 2002-03-25 00:00:00.0
	62	AX4610			C4 H10 O		74.122 1043 2002-03-25 00:00:00.0
	63	AX4611			C4 H5 N O2		99.0885 1044 2002-03-25 00:00:00.0
	64	AX4612			C4 H4 Cl N O2		133.534 1045 2002-03-25 00:00:00.0

from IsisDB

The screenshot shows the Inventory-LIMS interface. At the top, there is a navigation bar with links to Home, Biology, Chemistry, Xhibit, Xsite, MS, Data Analysis, Compound Screen, Inventory, and Monitor. The main header features the 'ACTIV X' logo and 'Inventory-LIMS'. Below this, there is a sub-header for 'Inventory' with tabs for Proteome, Probe, Smolecule, MolMarker, and Chembio. The 'InventoryView' tab is active. A table of chemical entries is displayed, with columns for Inventory, Probe, Axnumber, Name, Alias, Formula, Structure, and EntryIs. The table contains four rows of data, each with a chemical structure icon. A callout arrow points to the 'Structure' column with the text 'from IsisDB'. At the bottom, there is a copyright notice: 'Powered by the ActivX Bionformatics Team Copyright © 2002-2003 by ActivX, Inc'.



Home | Biology | Chemistry | Xhibit | Xsite | MS | Data Analysis | Compound Screen | Inventory | Monitor | Welcome Helge Logout

Xhibit-LIMS

Inventory Project Queue Report Document

New **XhibitPrime** Unstarted Ongoing Completed GelPlate

General

name

description

comment

number of timepoints

Click on "Proteomes", "Probes" or "Smolecules" button to select materials

Proteome

Plate Tube

Volume: uL

Probe

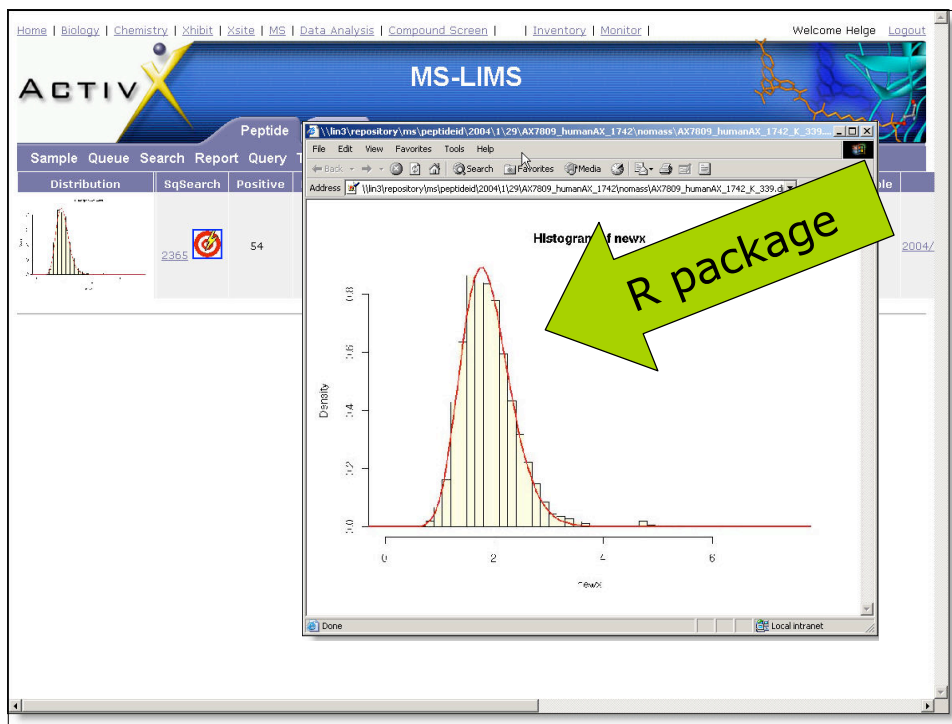
Plate Tube

Volume: uL

Smolecule

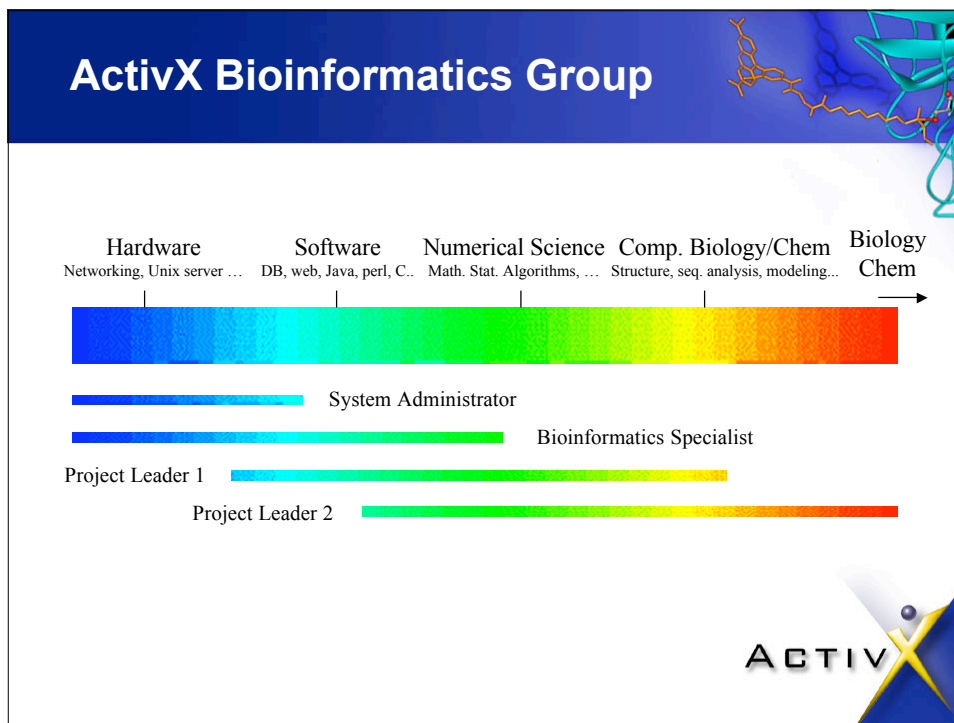
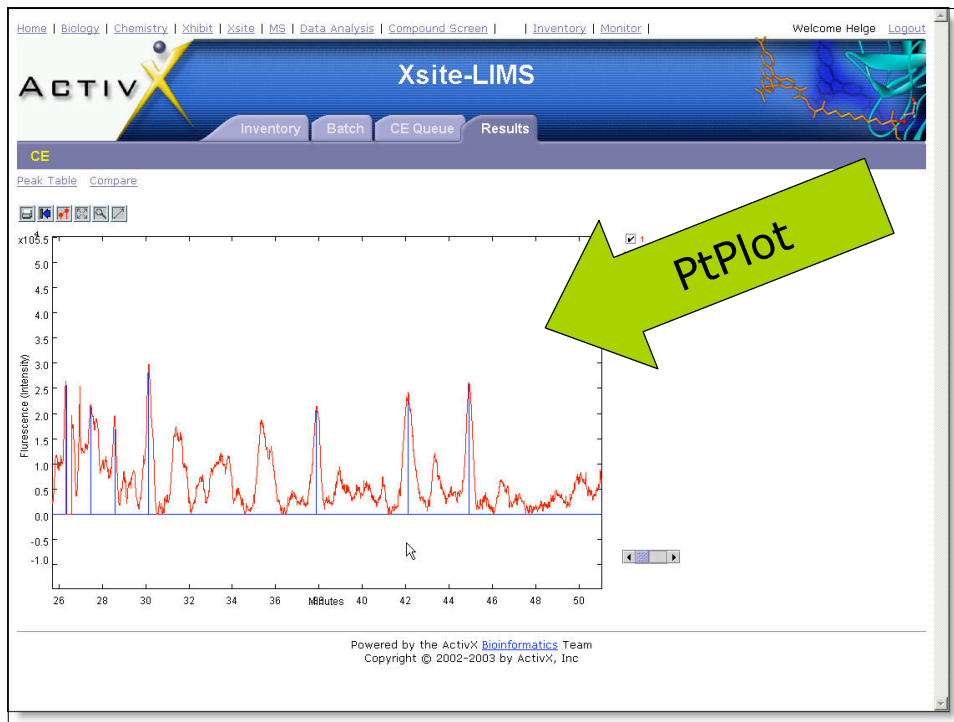
Plate Tube

Volume: uL



The screenshot shows the Xsite-LIMS interface. At the top, there is a navigation bar with links: Home | Biology | Chemistry | Xhibit | Xsite | MS | Data Analysis | Compound Screen | Inventory | Monitor | Welcome Helge | Logout. The main header displays the ACTIV logo and 'Xsite-LIMS'. Below this, there are tabs for 'Inventory', 'Batch', 'CE Queue', and 'Results'. A status bar shows 'New', 'Waiting', 'Current', and 'Completed'. The main area contains a 96-well plate layout with columns 1-12 and rows A-H. A 'Labelling' form is visible on the right, with fields for 'probeLabelConc' (value: uM), 'probeLabelBuffer' (value: 20% DMSO), and 'labelingTimeMinutes'. An 'Add Labelling Information' button is below the form. Below the form, there is a text block for 'Sample C3':
Sample C3
 12.0 ul of Animal-7 (Perry7:Vehicle Day 2, Heart, soluble) @ 12.0 mg/ml labeled with AX4596 @ 15.0 uM in 20% DMSO for 60.0 minutes

At the bottom, it says: Powered by the ActivX [Bioinformatics](#) Team
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Conclusions

- **Unique requirements for LIM Systems in Biotech**
- **Open-source framework models available**
- **Ease of development & integration**
- **Need for programming expertise in group**

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Acknowledgements

- **Joe Zou, Ph.D.**
- **Baohong Zhang, Ph.D.**
- **Xinghai Chen**
- **Jeff Leathers**

- **ActivX Biosciences, Inc.**

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