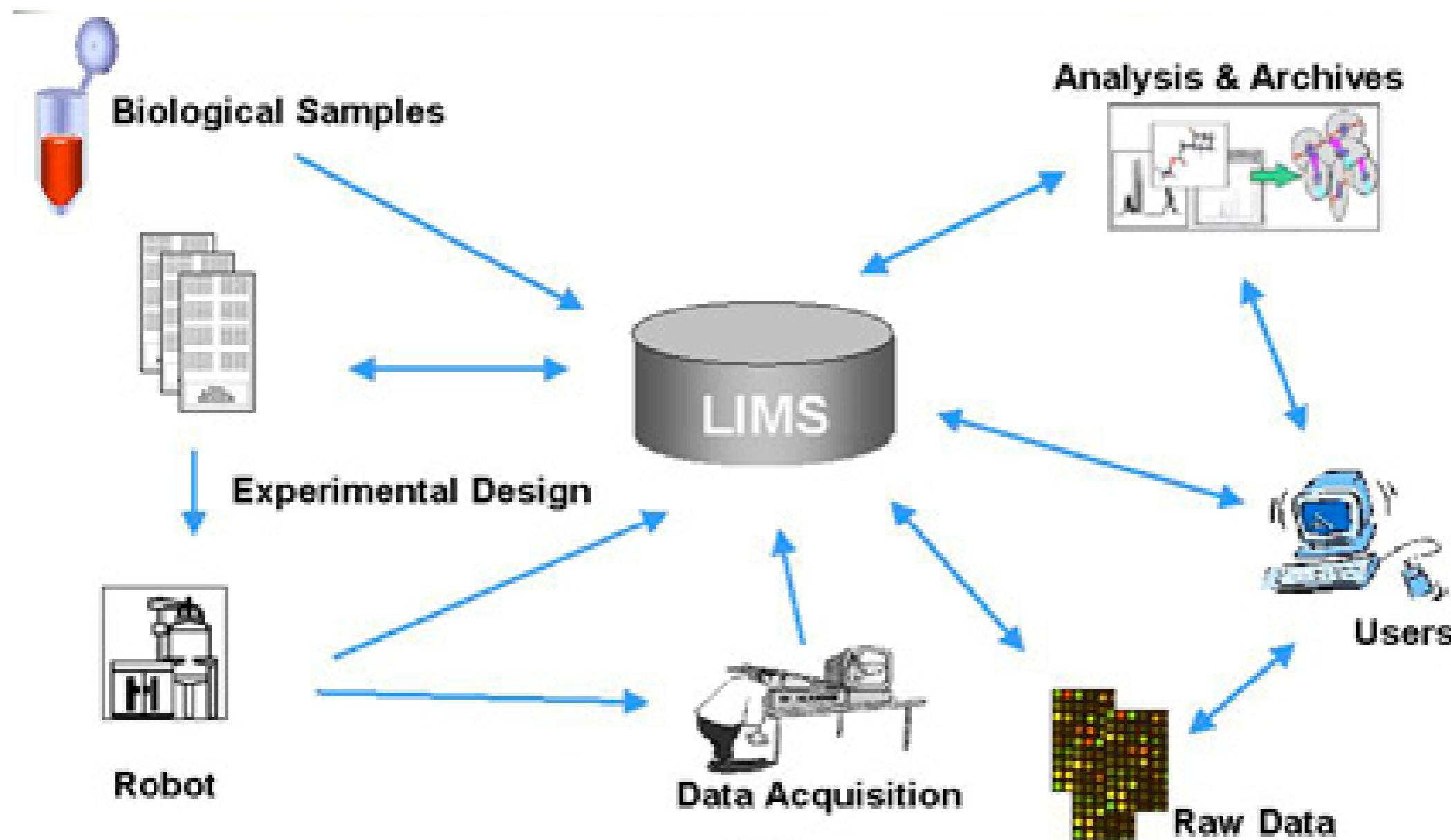


**LIMS**

# What is a LIMS?



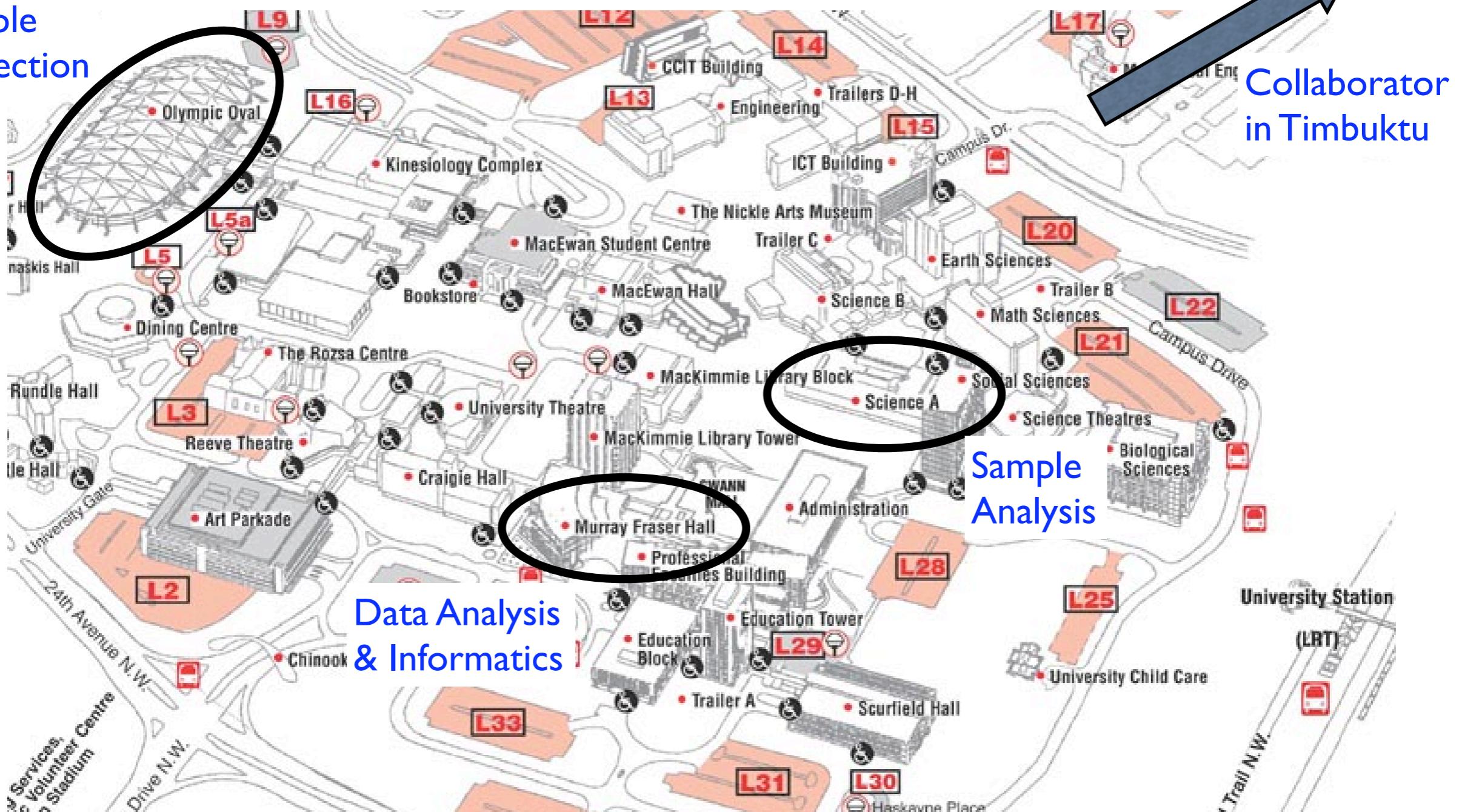
LIMS  
November 2003 - v.1.0

# LIMS

- LIMS = Laboratory Information Management System
- A data management system that allows tracking of laboratory samples from initial entry to the final reporting and analysis of results
- Useful for coordinating multi-lab or multi-investigator projects (proteomics, genomics, metabolomics, etc.)

# A Common Problem

Sample Collection



Data Analysis  
& Informatics

Sample  
Analysis

Collaborator  
in Timbuktu

# MetaboLIMS

# MetaboLIMS

- Web-based, portable, robust, and scalable LIMS designed to meet the high throughput processing and/or clinical needs of laboratories involved in -omics research
- Designed to be “generic” with some customizable features
- Very simple, intuitive interface
- Enforces user authentication to enhance security and access control to the system and its resources
- Integrated with the powerful search engines **BioSpider** and **PolySearch** that perform quick searches on a large variety of databases for chemical and/or biological information pertinent to any compounds of interest
- Includes a large database of well-annotated metabolites

# MetaboLIMS

- Compound and sample tracking
- Electronic notebook entry
- GANTT charting
- Instrument and meeting scheduling
- Text data entry
- Spectral trace or image entry
- Automated analysis and report generation
- Audit trail tracking
- Relational query searches
- NMR and MS spectral searches
- Automated compound annotation

# MetaboLIMS

**Main Page: View All Data - Microsoft Internet Explorer**

File Edit View Favorites Tools Help

Back Search Favorites Home Print Mail Links Address http://www.hmdb.ca/labm/jsp/home\_compound.jsp;jsessionid=4F843B0E23FFC7897CC4AAF06F5D66BD Go

**Gantt - Microsoft Internet Explorer**

File Edit View Favorites Tools Help

Back Search Favorites Home Print Mail Links Address http://www.hmdb.ca/~tomcat/gantt/cgi-bin/gantChart.cgi Go

Pop-up blocked. To see this pop-up or additional options click here...

Current Week		Weeks	09/04 to 09/11	09/11 to 09/18	09/18 to 09/25	09/25 to 10/02	10/02 to 10/09	10/09 to 10/16	10/16 to 10/23	10/23 to 10/30	10/30 to 11/06	11/06 to 11/13	11/13 to 11/20	11/20 to 11/27	11/27 to 12/04	12/04 to 12/11	12/11 to 12/18
<b>Tasks</b>																	
<ul style="list-style-type: none"> <li>Flag further fractionation using preparative HPLC</li> <li>Flag mass spec detection of 2nd-dimension fractions</li> <li>Flag getting feedbacks and likely repeating the processes to 1) fractionate more samples and 2) increase the purity of the fractions via additional fractionation using a different column.</li> <li>Flag separation using hplc</li> <li>Flag SOPs for working with CSF extraction</li> <li>Flag complete the addition of identified metabolites to bulletin/website</li> <li>Flag separations group begins NMR MS analysis</li> </ul>																	

**HMP Document Browser**

Forms/Posters Contact List HMP Milestones MSDB Search MS Search BioSpider HMDI

**HMP Data Browser**

-Metabolite Database- Metabolite Library BioSamples Identified Metabolites Users

**Enter New Metabolite**

2,862 results found, displaying 1 to 150

HMDB ID	Names
HMDB00001	1 Methylhistidine; 1 methyl L Histidine; 1 Methyl L histidine; 1 N Methyl L histidine; N1 Methyl L histidine; 1 Methylhistidine; 1 Methyl Histidine
HMDB00002	1,3 Diaminopropane; a,w Propanediamine; 1,3 Diarnpropane; 1,3 Propylenediamine; 1,3 Trimethylenediamine; 3 Aminopropylamine; TMEDA; Trimethylenediamine; 1,3 propanediamine; Propan

**Generate Compound Report - Microsoft Internet Explorer**

File Edit View Favorites Tools Help

Back Search Favorites Home Print Mail Links Address http://www.hmdb.ca/labm/jsp/mlims/Report.jsp Go

**Meeting Minutes - Microsoft Internet Explorer**

File Edit View Favorites Tools Help

Back Search Favorites Home Print Mail Links Address http://www.hmdb.ca/labm/servlet/MainServlet?handler=AllEventMinutes Go

**Meeting Minutes For MetaboLIMS**

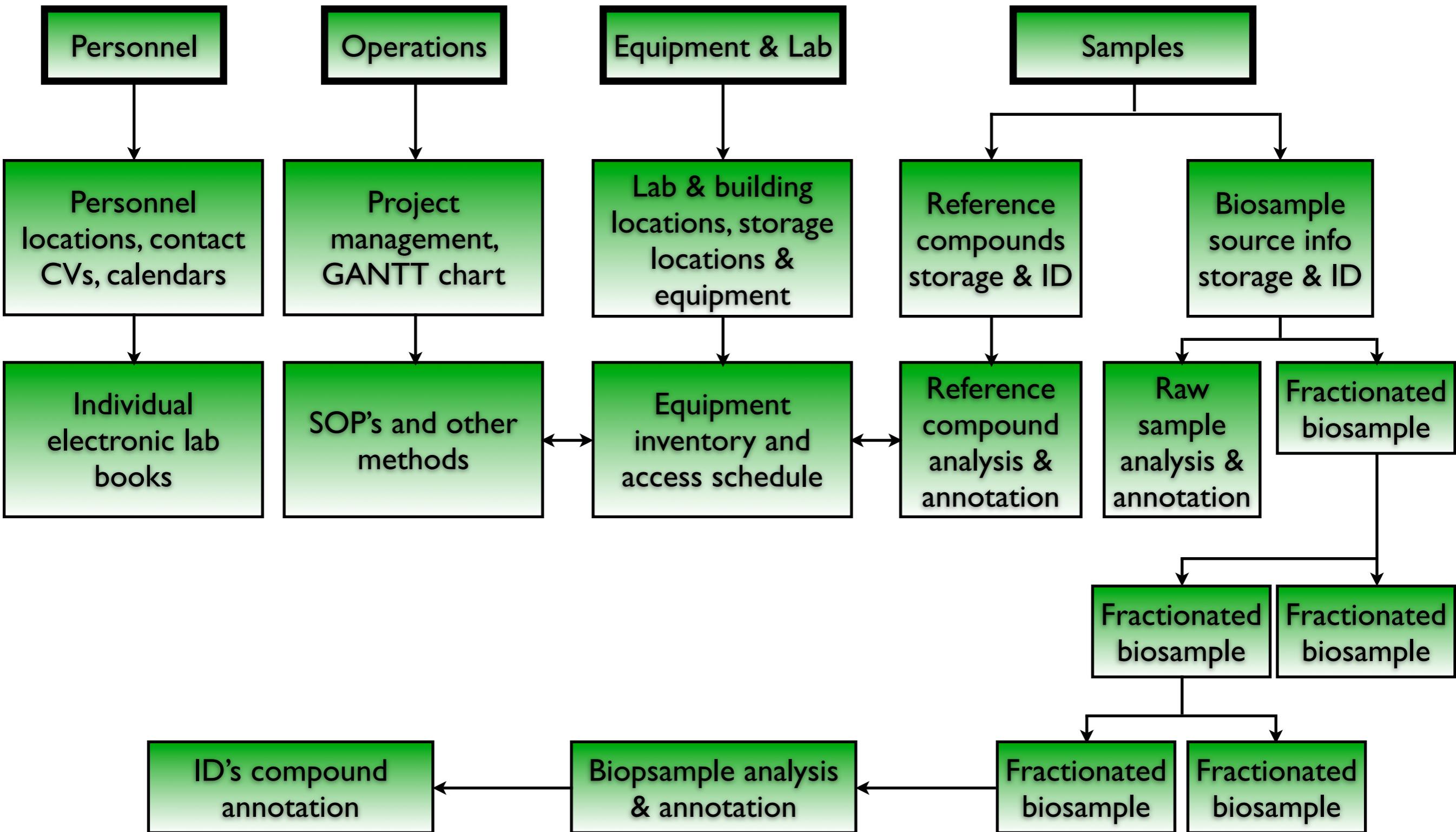
May 2006 June 2006

Su Mo Tu We Th Fr Sa	Su Mo Tu We Th Fr Sa
1 2 3 4 5 6	1 2 3
7 8 9 10 11 12 13	4 5 6 7 8 9 10
14 15 16 17 18 19 20	11 12 13 14 15 16 17
21 22 23 24 25 26 27	18 19 20 21 22 23 24
28 29 30 31	25 26 27 28 29 30

Previous 2 months Current 2 months Next 2 months Close window

Have Notes No Notes

# MetabolIMS Workflow



# Electronic Lab Book

- The electronic equivalent of a paper research notebook that allows users to easily create, organize, and manage all research data and documents online
- Allows information sharing
- Integrates seamlessly with the internet
- Cannot be misplaced, lost, or accidentally destroyed (if backed up)
- Allows data to be easily and efficiently searched
- Allows linked/embedded images and active hyperlinks to other websites

# Electronic Lab Book

The screenshot shows the MetaboLIMS web interface. At the top, there is a banner for the Human Metabolome Project (hmp) and Genome Canada/Alberta. Below the banner is a navigation menu with links for Home, Administration, Minutes, Planning, SOPs, Bulletin, Summary, Search, and Logout. The main content area is titled "HMP Document Browser" and contains links for Forms/Posters, Contact List, HMP Milestones, MSDB Search, MS Search, BioSpider, and HMDB. Below this is another section titled "HMP Data Browser" with links for -Metabolite Database-, Metabolite Library, BioSamples, Identified Metabolites, and Users. A large black arrow points from the word "Click" to the "Users" link in the HMP Data Browser menu. The bottom part of the screenshot shows a table titled "Enter New Metabolite" displaying results for "2,862 results found, displaying 1 to 150". The table includes columns for HMDB ID, Names, Chemical Formula, Molecular Weight (Da), CAS, and Export to HMDB. Several rows of metabolite data are listed, such as HMDB00001 (1 Methylhistidine; 1 methyl L Histidine; 1 Methyl L histidine; 1 N Methyl L histidine; N1 Methyl L histidine; L C7H11N3O2) and HMDB00002 (1,3 Diaminopropane; a,w Propanediamine; 1,3 Diamino n propane; 1,3 Propylenediamine; 1,3 Trimethylenediamine; 3 Aminopropylamine; TMEDA; Trimethylenediamine; 1,3 propanediamine; Propane 1,3 diamine).

HMDB ID	Names	Chemical Formula	Molecular Weight (Da)	CAS	Export to HMDB
HMDB00001	1 Methylhistidine; 1 methyl L Histidine; 1 Methyl L histidine; 1 N Methyl L histidine; N1 Methyl L histidine; L C7H11N3O2 1 Methylhistidine; 1 Methyl Histidine		169.08513	332-80-9	Yes
HMDB00002	1,3 Diaminopropane; a,w Propanediamine; 1,3 Diamino n propane; 1,3 Propylenediamine; 1,3 Trimethylenediamine; 3 Aminopropylamine; TMEDA; Trimethylenediamine; 1,3 propanediamine; Propane 1,3 diamine	C3H10N2	74.08440	109-76-2	Yes
HMDB00005	2 Ketobutyric acid; 2 oxo Butyric acid; b Ketobutyric acid; b Oxo n butyric acid; b Oxobutyric acid; b keto n Butyric acid; 2 Ketobutanic acid; 2 Oxo n butyric acid; 2 Oxobutanoic acid; 2 Oxobutyric acid; 3 Methylpyruvic acid; Propionylformic acid; 2 Oxo Butanoic acid; 2 Oxbutanoate; 2 oxobutanoic acid; propionyl Formic acid; Ketobutyrate; Oxobutyrate; methyl Pyruvic acid; alpha Keto n butyric acid; alpha Ketobutric acid; alpha Ketobutyric acid; alpha Oxo n butyric acid; alpha Oxobutyrate	C4H6O3	102.03169	600-18-0	Yes
HMDB00008	2 Hydroxybutyric acid; 2 hydroxy Butanoic acid; 2 hydroxy DL Butyric acid; a Hydroxybutyric acid; 2 Hydroxy n butyric acid; 2 Hydroxybutanoic acid; (RS) 2 Hydroxybutyric acid; a Hydroxy n butyrate; a Hydroxy n	C4H8O3	104.04734	600-15-	Yes

# Electronic Lab Book

The image shows two screenshots of the Electronic Lab Book interface. The left screenshot displays a 'Meeting Minutes' page from MetaboLIMS, featuring a calendar for May and June 2006, and a sidebar with project logos for hmp, MetaboLIMS, GenomeCanada, and GenomeAlt. The right screenshot shows a 'Project Manager Report' in a web-based word processor. It includes a toolbar with various icons, a section titled 'Project Manager Report:' containing text about a quarterly report and separations position, a 'Symposium:' section with a bulleted list of items, and a 'Project Updates' section. Arrows point from specific text elements to descriptive labels: one arrow points from the 'Hyperlink to SOPs' text to the 'Link' icon in the toolbar; another arrow points from the 'Paste tables & figures' text to the 'Table' and 'Image' icons in the toolbar.

Common calendar view for all registered project staff

Hyperlink to SOPs

Paste tables & figures

Return to Calendar    <<< Previous Day    Next Day >>>    Close Window

User : minutes    E-Lab Book    Date: 12/10/2005

Edit Mode    Times New Roman    3 (12 Pt)    B I U S x<sub>2</sub> x<sup>2</sup>

Project Manager Report:

Quarterly report: Thank you to all of the PI's who have provided me with their technical update. PI approval. For those who have not yet done so, please get it to me ASAP. I will also need to HMDB as of September 30.

Separations Position: Lisa Nikolai has been hired by David and will be starting October 17.

SAB meeting: Agenda needs to be finalized. Lori will circulate to SAB members and Genome Prairie when set. The project presentations and who will be presenting and what the format will be of the presentations. I would recommend that power point be used for the presentations. Lori by October 24 so hard copies can be made for the SAB meeting.

Symposium:

- All speakers are confirmed and I have attached a working agenda for the symposium.
- So far I have indications of 1 poster from the Project (Erik's). Please let me know if you plan on submitting a poster.
- I also need all project members to confirm their attendance at the symposium (as this will also confirm the number of people attending).
- I have also printed up conference posters that I would ask that you all post in your buildings. If you need more posters, please let me know.
- Speaker's dinner: I (and Chenomx) are trying to get Varian to sponsor the dinner for the speakers on Monday night. We will be having the dinner after the lunch or the speaker's dinner. If there is anyone you think I should approach for funding the conference, or if you know of anyone who might be interested, please let me know.

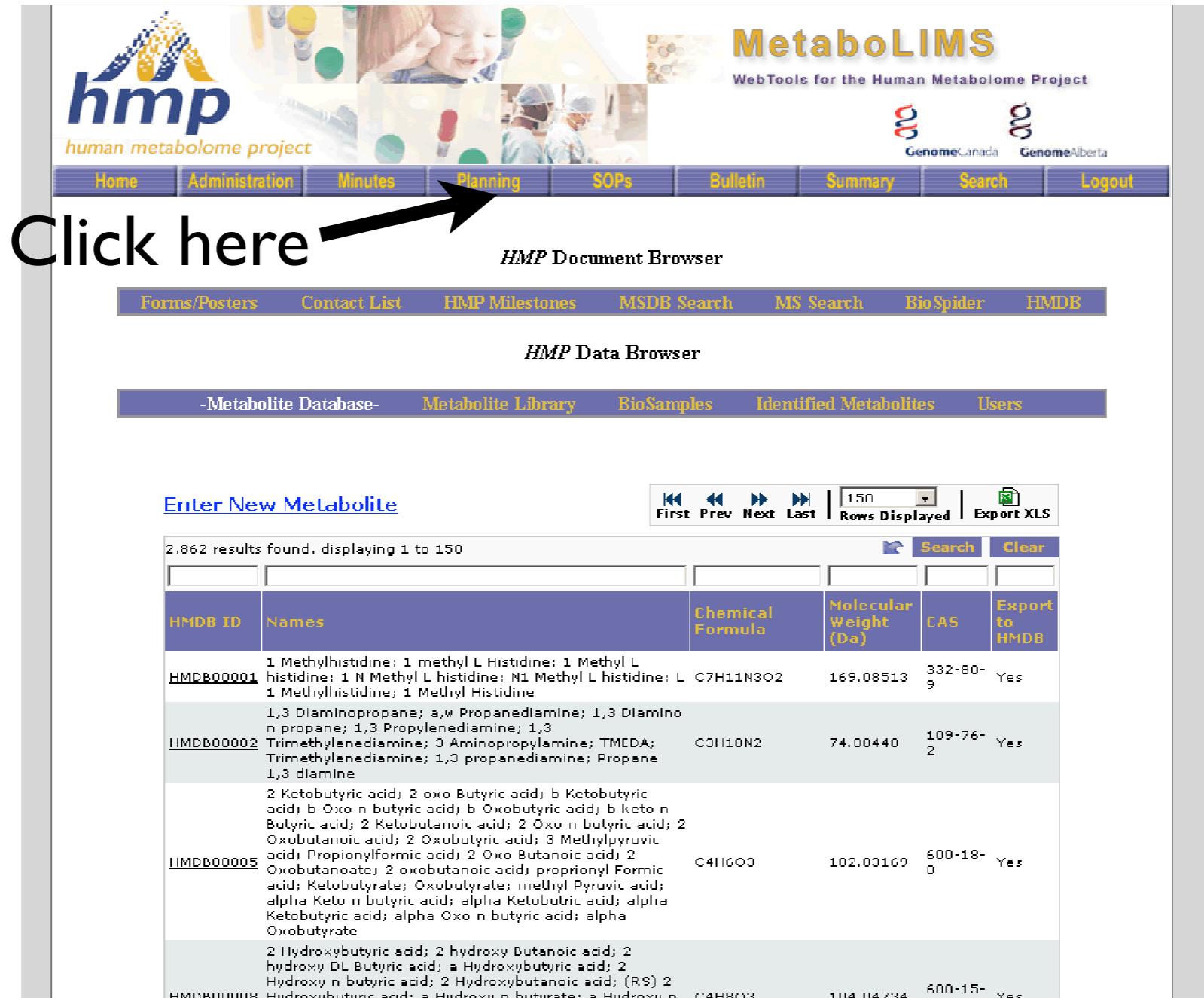
Project Updates

Li lab update - Mulu Gebre

Submit    Delete    Clear

A web-like version of MS word

# Project Planning



Click here →

**MetaboLIMS**  
WebTools for the Human Metabolome Project

hmp  
human metabolome project

Home Administration Minutes Planning SOPs Bulletin Summary Search Logout

HMP Document Browser

Forms/Posters Contact List HMP Milestones MSDB Search MS Search BioSpider HMDB

HMP Data Browser

- Metabolite Database - Metabolite Library BioSamples Identified Metabolites Users

Enter New Metabolite

Enter New Metabolite					
2,862 results found, displaying 1 to 150					
HMDB ID	Names	Chemical Formula	Molecular Weight (Da)	CAS	Export to HMDB
HMDB00001	1 Methylhistidine; 1 methyl L Histidine; 1 Methyl L histidine; 1 N Methyl L histidine; N1 Methyl L histidine; L-C7H11N3O2	169.08513	332-80-9	Yes	
HMDB00002	1,3 Diaminopropane; a,w Propanediamine; 1,3 Diamino n-propane; 1,3 Propylenediamine; 1,3 Trimethylenediamine; 3 Aminopropylamine; TMEDA; Trimethylenediamine; 1,3 propanediamine; Propane 1,3 diamine	C3H10N2	74.08440	109-76-2	Yes
HMDB00005	2 Ketobutyric acid; 2 oxo Butyric acid; b Ketobutyric acid; b Oxon butyric acid; b Oxobutyric acid; b keto n-Butyric acid; 2 Ketobutanoic acid; 2 Oxo n butyric acid; 2 Oxobutanoic acid; 2 Oxobutyric acid; 3 Methylpyruvic acid; Propionylformic acid; 2 Oxo Butanoic acid; 2 Oxobutanoate; 2 oxobutanoic acid; propionyl Formic acid; Ketobutyrate; Oxobutyrate; methyl Pyruvic acid; alpha Keto n butyric acid; alpha Ketobutric acid; alpha Ketobutyric acid; alpha Oxo n butyric acid; alpha Oxobutyrate	C4H6O3	102.03169	600-18-0	Yes
HMDB00008	2 Hydroxybutyric acid; 2 hydroxy Butanoic acid; 2 hydroxy DL Butyric acid; a Hydroxybutyric acid; 2 Hydroxy n butyric acid; 2 Hydroxybutanoic acid; (RS) 2-Hydroxybutyric acid; a Hydroxy n butyrate; a Hydroxy n	C4H8O3	104.04734	600-15-	Yes

# Project Planning (GANTT)

- Includes a simple, easy-to-use GANTT charting feature that monitors, assigns, and redistributes the tasks as and when required
  - Helps determine the resources needed, the order of and dependencies between the tasks which are useful for planning and scheduling projects

# Shareable Calendar

- Allows users to manage their schedules online and share them with all or only “designated, privileged” users

The screenshot shows a web-based calendar interface for the Human Metabolome Project (HMP). The top header includes the HMP logo, a photograph of laboratory equipment and researchers, and logos for Genome Canada and Genome Alberta. Below the header, a navigation bar offers links to 'Back to Calendar', '<<< Previous Day', 'Next Day >>>', and 'Close Window'. The main content area displays a 24-hour schedule grid for 'Person: adampeng, Friday March 7, 2008'. The grid is organized into two columns of 12 time slots each, from 0800-0830 to 1330-1400. Each slot contains a checkbox for booking. Above the grid, a legend identifies the colors: light gray for 'Vacant', orange for 'One-Time', red for 'Daily', green for 'Weekly', and blue for 'Monthly'. Buttons for 'Check All' and 'Uncheck All' are also present. At the bottom of the grid, there are fields for 'Frequency' (set to 'This day only') and 'Repeat until(dd/mm/yyyy)', along with a text input for 'Reason for booking (please be brief)' and a checkbox for 'Travel/Vacation'.

# MetaboLIMS

# Metabolite Page

“instant”  
text search

Click

The screenshot shows the MetaboLIMS Metabolite Page. At the top, there's a banner for the Human Metabolome Project (hmp) and Genome Canada/Alberta. Below the banner is a navigation menu with links: Home, Administration, Minutes, Planning, SOPs, Bulletin, Summary, Search, and Logout. The main content area has two tabs: 'HMP Document Browser' and 'HMP Data Browser'. Under 'HMP Document Browser', there are links for Forms/Posters, Contact List, HMP Milestones, MSDB Search, MS Search, BioSpider, and HMDB. Under 'HMP Data Browser', there are links for -Metabolite Database-, Metabolite Library, BioSamples, Identified Metabolites, and Users. The central part of the page is a table titled 'Enter New Metabolite'. The table header includes columns for HMDB ID, Names, Chemical Formula, Molecular Weight (Da), CAS, and Export to HMDB. The table body contains several rows of metabolite data. Two arrows point to the search bar at the top of the table and the first row of the table.

HMDB ID	Names	Chemical Formula	Molecular Weight (Da)	CAS	Export to HMDB
HMDB00001	1 Methylhistidine; 1 methyl L Histidine; 1 Methyl L histidine; 1 N Methyl L histidine; N1 Methyl L histidine; L-C7H11N3O2 1 Methylhistidine; 1 Methyl Histidine		169.08513	332-80-9	Yes
HMDB00002	1,3 Diaminopropane; a,w Propanediamine; 1,3 Diamino n-propane; 1,3 Propylenediamine; 1,3 Trimethylenediamine; 3 Aminopropylamine; TMEDA; Trimethylenediamine; 1,3 propanediamine; Propane 1,3 diamine	C3H10N2	74.08440	109-76-2	Yes
HMDB00005	2 Ketobutyric acid; 2 oxo Butyric acid; b Ketobutyric acid; b Oxo n butyric acid; b Oxobutyric acid; b keto n Butyric acid; 2 Ketobutanoic acid; 2 Oxo n butyric acid; 2 Oxobutanoic acid; 2 Oxobutyric acid; 3 Methylpyruvic acid; Propionylformic acid; 2 Oxo Butanoic acid; 2 Oxobutanate; 2 oxobutanoic acid; propionyl Formic acid; Ketobutyrate; Oxobutyrate; methyl Pyruvic acid; alpha Keto n butyric acid; alpha Ketobutyric acid; alpha Ketobutyric acid; alpha Oxo n butyric acid; alpha Oxobutyrate	C4H6O3	102.03169	600-18-0	Yes
HMDB00008	2 Hydroxybutyric acid; 2 hydroxy Butanoic acid; 2 hydroxy DL Butyric acid; a Hydroxybutyric acid; 2 Hydroxy n butyric acid; 2 Hydroxybutanoic acid; (RS) 2 Hydroxybutyric acid; a Hydroxy n butyrate; a Hydroxy n	C4H8O3	104.04734	600-15-	Yes

# MetaboLIMS

## MetaboCard

Metabolite data {

BioSpider

**Dimethylmalonic acid (HMDB02001)**

Chemical Properties (18/33) Completed	Concentrations (1/16) Completed	Other Links (3/9) Completed	SimCell No Data	Biological Data No Data	Acquisition Info No Data	C NMR No Data	2D HSQC No Data	H NMR (Sykes) No Data	H NMR (Wishart) No Data	Mass Spec No Data
---	---------------------------------------	-----------------------------------	--------------------	----------------------------	-----------------------------	------------------	--------------------	--------------------------	----------------------------	----------------------

Chemical Properties

Accession # D02001  
Creation Date 2006-05-22 15:17:31  
Common Name Dimethylmalonic acid  
Not Available

Descriptions

Synonyms  
2,2-Dimethylmalonic acid;  
2,2-Propanedcarboxylic acid;  
2,2-dimethylmalonic acid (ACD/Name 4.0);  
Malonic acid, dimethyl-; Malonic acid,  
dimethyl- (8CI); Propanedioic acid,  
dimethyl-; propanedioic acid dimethyl

Chemical IUPAC Name 2,2-dimethylpropanedioic acid  
Chemical Formula C5H8O4  
Chemical Structure (Zoom) [Browse...](#)  
Chemical Structure (Thumbnail) [Browse...](#)  
Molecular Weight (g/mol) 132.04227  
Average Molecular Weight (g/mol) 132.11462  
Smiles String CC(C)(C(=O)O)C(=O)O  
CAS Number 595-46-0

↑ Data status “bar”

↓ Scroll down

# MetaboLIMS

## MetaboCard

The MetaboCard interface integrates experimental data with chemical structures and spectral analysis.

**Experimental Data:**

- Sample Operator: Technician\_in\_Wishart's\_Lab
- Collection Date: Apr 18 2006
- Sample Preparation Protocol: Dissolution of Standard Samples for NMR Protocol SOP 012 V1.doc
- Sample Concentration (mM): 50
- Sample Mass: 5.9 mg
- Instrument Manufacturer: Varian
- Spectrometer Freq (MHz): 500
- NMR Data Collection Protocol: Conducting 'presat' and 'NOESY' 1D Experiments Protocol SOP 013 v1.doc
- 1H NMR Spectra: 041031\_P00\_04\_IS\_1DP\_noesy.png, 041031\_P00\_04\_IS\_1DP\_presat.png
- FIDS For NMR Spectra: 041031\_P00\_04\_IS\_1DP\_noesy.zip, 041031\_P00\_04\_IS\_1DP\_presat.zip
- Peak List For NMR Spectra: 041031\_P00\_04\_IS\_1DP.txt
- Assignment For NMR Spectra: 041031\_P00\_04\_IS\_1DP\_Assigned.pdf
- Spectra Deposit Date: Apr 27 2006
- Spectra: Excellent

**Spectral Analysis:**

Full 1H NMR Spectrum (500 MHz in H<sub>2</sub>O):

- Chemical Shift (ppm): 10 to -1.
- Peak Labels: DMSO(6.8), HDOWater(4.8), H2O(4.7), M01(4.2), M02(4.0), M03(3.8), M04(3.6), M05(3.5), M06(3.4), M07(3.3), M08(3.2), M09(3.1), M10(3.0), M11(2.9), M12(2.8), M13(2.7), M14(2.6), M15(2.5), M16(2.4), M17(2.3), M18(2.2), M19(2.1), M20(2.0), M21(1.9), M22(1.8), M23(1.7), M24(1.6), M25(1.5), M26(1.4), M27(1.3), M28(1.2), M29(1.1), M30(1.0), M31(0.9), M32(0.8), M33(0.7), M34(0.6), M35(0.5), M36(0.4), M37(0.3), M38(0.2), M39(0.1), DSS(0.0).

**Chemical Structure:**

1-Methylhistidine (HMDB00001)

Chemical structure diagram showing atoms labeled 1 through 12. Atoms 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and 12 are explicitly numbered. Atoms 1, 2, and 3 are part of the imidazole ring. Atom 4 is the nitrogen atom. Atom 5 is the carbon atom bonded to the imidazole ring. Atom 6 is the methyl group. Atom 7 is the nitrogen atom bonded to the side chain. Atom 8 is the carbonyl carbon. Atom 9 is the amide nitrogen. Atom 10 is the carbonyl oxygen. Atom 11 is the amide hydrogen. Atom 12 is the hydroxyl hydrogen.

**Table of Multiplets:**

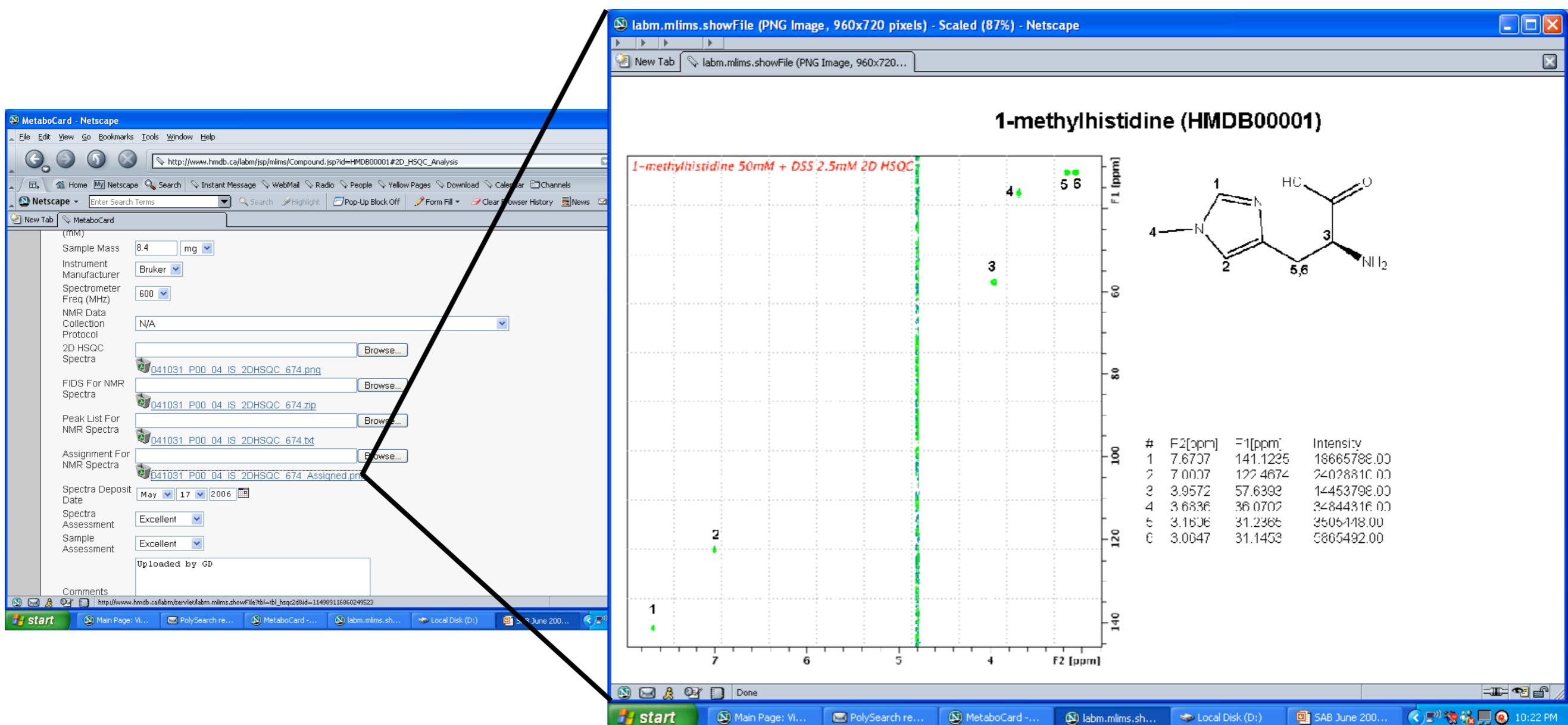
No.	Chem. Shift (ppm)	Int.	Type	J (Hz)	Atom(s)	Multiplet	(ppm)
1	3.11	2	m	-	7	M05	(3.02, 3.21)
2	3.68	3	s	-	8	M04	(3.67, 3.71)
3	3.65	1	dd	7.65, 4.67	9	M03	(3.62, 4.01)
4	7.03	1	s	-	4	M02	(6.98, 7.02)
5	7.68	1	s	-	2	M01	(7.65, 7.75)

**Table of Assignments:**

No.	Atom	Exp. Shift (ppm)	Multiplet
1	7	3.11	M05
2	6	3.68	M04
3	8	3.65	M03
4	4	7.03	M02
5	2	7.68	M01

# MetaboLIMS

## MetaboCard



# Auto-annotate Metabolite Data with BioSpider

Click here

BioSpider

Dimethylmalonic acid (HMDB02001)

Chemical Properties (18/33) Completed	Concentrations (1/16) Completed	Other Links (3/9) Completed	SimCell No Data	Biological Data No Data	Acquisition Info No Data	C NMR No Data	2D HSQC No Data	H NMR (Sykes) No Data	H NMR (Wishart) No Data	Mass Spec No Data
---	---------------------------------------	-----------------------------------	--------------------	----------------------------	-----------------------------	------------------	--------------------	--------------------------	----------------------------	----------------------

Chemical Properties

Accession # 02001

Creation Date 2006-05-22 15:17:31

Common Name Dimethylmalonic acid

Descriptions Not Available

Synonyms 2,2-Dimethylmalonic acid;  
2,2-Propanedicarboxylic acid;  
2,2-dimethylmalonic acid (ACD/Name 4.0);  
Malonic acid, dimethyl-; Malonic acid,  
dimethyl- (8CI); Propanedioic acid,  
dimethyl-; propanedioic acid dimethyl

Chemical IUPAC Name 2,2-dimethylpropanedioic acid

Chemical Formula C5H8O4

Chemical Structure (Zoom)

Chemical Structure (Thumbnail)

Molecular Weight (g/mol) 132.04227

Average Molecular Weight (g/mol) 132.11462

Smiles String CC(C)(C=O)O)C(=O)O

CAS Number 595-46-0

# Dual Display helps Annotation

 BioSPIDER

[Expand all](#) [Collapse all](#) [Only allow one expanded element](#)

**Dimethylmalonic acid (HMDB02001)**

<a href="#">Chemical Properties</a>	<a href="#">Concentrations</a>	<a href="#">Other Links</a>	<a href="#">Biological Data</a>
(18/33) Completed	(1/16) Completed	(3/9) Completed	No Data

LIMS BioSpider

▼ Chemical Properties

Accession #	02001	
Creation Date	2006-05-22 15:17:31	
Common Name	Dimethylmalonic acid	
	Not Available	
Descriptions		
Synonyms	2,2-Dimethylmalonic acid; 2,2-Propanedicarboxylic acid; 2,2-dimethylmalonic acid (ACD/Name 4.0); Malonic acid, dimethyl-; Malonic acid, dimethyl- (8CI); Propanedioic acid, dimethyl-; propanedioic acid dimethyl	
Chemical IUPAC Name	2,2-dimethylpropanedioic acid	
Chemical Formula	C5H8O4	
Molecular Weight (g/mol)	132.04227	
Average		

# Sample Tracking / Entry

The screenshot shows the MetaboLIMS web application interface. At the top, there is a banner for the Human Metabolome Project (hmp) and the MetaboLIMS project, which is described as "Web Tools for the Human Metabolome Project". Below the banner is a navigation menu with links to Home, Administration, Minutes, Planning, SOPs, Bulletin, Summary, Search, and Logout. A large arrow points from the text "Click here" to the "HMP Data Browser" link in the menu.

The main content area is titled "HMP Document Browser" and "HMP Data Browser". Below these titles is a sub-menu with links to Forms/Posters, Contact List, HMP Milestones, MSDB Search, MS Search, BioSpider, and HMDB. The "HMP Data Browser" section is currently active, indicated by a blue background. It features a table titled "Enter New Metabolite" displaying results for "2,862 results found, displaying 1 to 150". The table columns include HMDB ID, Names, Chemical Formula, Molecular Weight (Da), CAS, and Export to HMDB. The first few rows of data are as follows:

HMDB ID	Names	Chemical Formula	Molecular Weight (Da)	CAS	Export to HMDB
<a href="#">HMDB00001</a>	1 Methylhistidine; 1 methyl L Histidine; 1 Methyl L histidine; 1 N Methyl L histidine; N1 Methyl L histidine; L C7H11N3O2 1 Methylhistidine; 1 Methyl Histidine		169.08513	332-80-9	Yes
<a href="#">HMDB00002</a>	1,3 Diaminopropane; a,w Propanediamine; 1,3 Diamino n propane; 1,3 Propylenediamine; 1,3 Trimethylenediamine; 3 Aminopropylamine; TMEDA; Trimethylenediamine; 1,3 propanediamine; Propane 1,3 diamine	C3H10N2	74.08440	109-76-2	Yes
<a href="#">HMDB00005</a>	2 Ketobutyric acid; 2 oxo Butyric acid; b Ketobutyric acid; b Oxo n butyric acid; b Oxobutyric acid; b keto n Butyric acid; 2 Ketobutanoic acid; 2 Oxo n butyric acid; 2 Oxobutanoic acid; 2 Oxobutyric acid; 3 Methylpyruvic acid; Propionylformic acid; 2 Oxo Butanoic acid; 2 Oxobutanoate; 2 oxobutanoic acid; propionyl Formic acid; Ketobutyrate; Oxobutyrate; methyl Pyruvic acid; alpha Keto n butyric acid; alpha Ketobutric acid; alpha Ketobutyric acid; alpha Oxo n butyric acid; alpha Oxobutyrate	C4H6O3	102.03169	600-18-0	Yes
<a href="#">HMDB00008</a>	2 Hydroxybutyric acid; 2 hydroxy Butanoic acid; 2 hydroxy DL Butyric acid; a Hydroxybutyric acid; 2 Hydroxy n butyric acid; 2 Hydroxybutanoic acid; (RS) 2 Hydroxibutyric acid; a Hydroxy n butyrate; a Hydroxy n	C4H8O3	104.04734	600-15-	Yes

# MetaboLIMS

## Sample Tracking

  **MetaboLIMS**  
WebTools for the Human Metabolome Project

View Sample 05112202\_B01\_F014

null

ID 05112202\_B01\_F014  
Responsible User Lisa Nikolai  
Sample Acquisition Date 2005-12-16  
Location Biosti -> B322 -> Refrigerator  
Source Blood  
Sample Type Fraction  
Amount 1.0 mL  
Description Gradient details: 100:0 (10) -> 90:10 15(5) -> 5(5) A/B where: A=0.1%TFA in water B=AcN w 0.1% TFA flow=2ml/min stoptime=40mins This is shorthand for: hold 0% B (AcN w 0.1% TFA)for 10 minutes increase to 10% B at 25 minutes hold at 10% B for 5 minutes decrease to 0% B at 35 minutes hold at 0% B for 5 minutes

[View Analysis from Ultrasphere C18](#)  
[View Analysis from Varian Unity Inova 500MHz](#)  
[View Analysis from Varian Unity Inova 500MHz](#)  
[View Analysis from Varian Unity Inova 500MHz](#)

**Identified Compounds**

ID	Experiment	Type	Value	Unit
----	------------	------	-------	------

Available Actions

Sample used up?   
# Fractions 2  
Fraction Size 0.0 mL

Navigation [Home](#) [Browse All Samples](#) [Compounds](#) [Add a Sample](#)  [Search Samples](#)

# Audit Trail

- Tracks progress by logging user activities in the system
- Logs are searchable by using a simple, intuitive interface

The screenshot shows a web-based application interface for the Human Metabolome Project (HMP). At the top, there is a navigation bar with links for Home, Administration, Minutes, Planning, SOPs, Bulletin, Summary, Search, and Logout. Below this is another navigation bar specific to the HMP Document Browser, with links for Forms/Posters, Contacts, Milestones, Searches, Mass Calc, Stats, BioSpider, and HMDB.

The main content area is titled "HMP Document Browser" and contains a sub-section titled "HMP Data Browser". This section includes a navigation bar with links for Metabolite Database, Metabolite Library, BioSamples, Identified Metabolites, Users, and -Audit Trail-. Below this is a search interface with a "Search" input field and a "Search" button. A message indicates "10,000 results found, displaying 1 to 150".

The bottom half of the screenshot displays a table titled "Audit Trail" with the following columns: HMDB ID, User, Date, Modification Type, Table, Field, Former Value, and Modified Value. The table lists several audit log entries:

HMDB ID	User	Date	Modification Type	Table	Field	Former Value	Modified Value
HMDB00318	dan	Mon Apr 14 09:53:18 update MDT 2008	tbl_concentrations comment			(24 months-18 years)	
HMDB00318	dan	Mon Apr 14 09:54:17 update MDT 2008	tbl_concentrations comment			(adult)	
HMDB00315	dan	Mon Apr 14 10:47:36 update MDT 2008	tbl_concentrations comment			(umbilical cord blood, term) uM (umbilical cord blood, term)	
HMDB00752	dan	Thu Apr 17 10:29:19 update MDT 2008	tbl_concentrations comment			2-6 years: 1 umol/mmol creatinine	
		Thu Apr 17				5.9-28.3 nmol/mmol_creatinine	

# MetaboLIMS Reporting

The screenshot shows the MetaboLIMS reporting interface. At the top, there is a banner for the Human Metabolome Project (hmp) featuring a smiling baby and laboratory glassware. The banner includes the text "MetaboLIMS WebTools for the Human Metabolome Project" and logos for Genome Canada and Genome Alberta. Below the banner is a navigation menu with links: Home, Administration, Minutes, Planning, SOPs, Bulletin, Summary (which has a large black arrow pointing to it), Search, and Logout.

In the center, there is a section titled "Click here" followed by "HMP Document Browser". Below this is another section titled "HMP Data Browser" with tabs for Metabolite Database, Metabolite Library, BioSamples, Identified Metabolites, and Users.

The main content area displays a table titled "Enter New Metabolite" with 2,862 results found, displaying 1 to 150. The table columns include HMDB ID, Names, Chemical Formula, Molecular Weight (Da), CAS, and Export to HMDB. The table shows several rows of metabolite data, such as:

HMDB ID	Names	Chemical Formula	Molecular Weight (Da)	CAS	Export to HMDB
HMDB000001	1 Methylhistidine; 1 methyl L Histidine; 1 Methyl L histidine; 1 N Methyl L histidine; N1 Methyl L histidine; L-C7H11N3O2 1 Methylhistidine; 1 Methyl Histidine		169.08513	332-80-9	Yes
HMDB000002	1,3 Diaminopropane; a,w Propanediamine; 1,3 Diamino n propane; 1,3 Propylenediamine; 1,3 Trimethylenediamine; 3 Aminopropylamine; TMEDA; Trimethylenediamine; 1,3 propanediamine; Propane 1,3 diamine	C3H10N2	74.08440	109-76-2	Yes
HMDB000005	2 Ketobutyric acid; 2 oxo Butyric acid; b Ketobutyric acid; b Oxo n butyric acid; b keto n Butyric acid; 2 Ketobutanoic acid; 2 Oxo n butyric acid; 2 Oxobutanoic acid; 2 Oxobutyric acid; 3 Methylpyruvic acid; Propionylformic acid; 2 Oxo Butanoic acid; 2 Oxobutanoate; 2 oxobutanoic acid; propionic Formic acid; Ketobutyrate; Oxobutyrate; methyl Pyruvic acid; alpha Keto n butyric acid; alpha Ketobuteric acid; alpha Ketobutyric acid; alpha Oxo n butyric acid; alpha Oxobutyrate	C4H6O3	102.03169	600-18-0	Yes
HMDB000008	2 Hydroxybutyric acid; 2 hydroxy Butanoic acid; 2 hydroxy DL Butyric acid; a Hydroxybutyric acid; 2 Hydroxy n butyric acid; 2 Hydroxybutanoic acid; (RS)-2-Hydroxybutyric acid; a Hydroxy n butyrate; a Hydroxy n	C4H8O3	104.04734	600-15-	Yes

# MetaboLIMS

# Report Generator

Generate Compound Report - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Favorites Address  Go

**hmp** *human metabolome project*

**MetaboLIMS**  
WebTools for the Human Metabolome Project

**Columns to Display in Report:**

Sort by Ascending Order in HMDB ID Display 20

<input checked="" type="checkbox"/> HMDB ID	<input type="checkbox"/> Chemical Structure (Image)	<input checked="" type="checkbox"/> Compound Status
<input type="checkbox"/> Metabolite ID	<input checked="" type="checkbox"/> Chemical Formula	<input checked="" type="checkbox"/> Supplier
<input checked="" type="checkbox"/> Common Name	<input type="checkbox"/> Molecular Weight	<input checked="" type="checkbox"/> H NMR Spectra (Sykes)
<input type="checkbox"/> IUPAC Name	<input type="checkbox"/> logP	<input checked="" type="checkbox"/> H NMR Spectra (Wishart)
<input checked="" type="checkbox"/> CAS	<input type="checkbox"/> H <sub>2</sub> O Solubility	<input checked="" type="checkbox"/> C NMR Spectra
<input type="checkbox"/> InChi #	<input type="checkbox"/> H <sub>2</sub> O Solubility (Predicted)	<input type="checkbox"/> Mass Spec Spectra
	<input type="checkbox"/> State	<input type="checkbox"/> 2D_HSQC Spectra
<input type="checkbox"/> Clive's Summary	<input checked="" type="checkbox"/> Default Summary	

# NMR Search

- Perform custom searches on <sup>1</sup>H, <sup>13</sup>C, Tocsy, and 2D HSQC data in the NMR spectral databases
- Results can be filtered and searched, then exported to Excel format easily

NMR Spectral Search Submit [Help] 

Search Type	All												
Spectral Database	1D_1H_NMR												
Top Matches Returned	100												
Chemical Shift Type	1H N/A												
Chemical Shift Tolerance (+/-)	0.03 0												
Chemical Shift Library	<table border="1"><tr><td>6.00</td><td>6.00</td></tr><tr><td>5.12</td><td>5.12</td></tr><tr><td>4.66</td><td>4.66</td></tr><tr><td>4.59</td><td>4.59</td></tr><tr><td>8.32</td><td>8.32</td></tr><tr><td>8.13</td><td>8.13</td></tr></table>	6.00	6.00	5.12	5.12	4.66	4.66	4.59	4.59	8.32	8.32	8.13	8.13
6.00	6.00												
5.12	5.12												
4.66	4.66												
4.59	4.59												
8.32	8.32												
8.13	8.13												
Submit [Help]													

Search Result First Prev Next Last 100 Rows Displayed Export XLS

100 results found, displaying 1 to 100				
HMDB ID	Name	Peaklist	Category	Score
HMDB01473	Dihydroxyacetone phosphate	View	predicted	3/3
HMDB00034	Adenine	View	experimental	2/2
HMDB00034	Adenine	View	predicted	2/3
HMDB00119	Glyoxylic acid	View	experimental	1/2
HMDB03163	6-Chloroguanine	View	predicted	1/2
HMDB00123	Glycine	View	predicted	1/2
HMDB00956	Tartaric acid	View	predicted	1/2
HMDB01352	Hydroxypyruvic acid	View	predicted	1/2
HMDB01219	Chlordecone alcohol	View	predicted	1/2
HMDB00058	Cyclic AMP	View	predicted	4/9

Done

# GC/MS-MS Search

**GC/MS Search**

Perform : GC/MS Search

GC/MS Search

Find Metabolites

Parent Mass of Derivatized Compound: 174.1 (Da) [234 Da for L-Lactic acid]

Parent Mass Tolerance ( $\pm$ ): 0.1 (Da)

Retention Index: 1072

Tolerance for Retention Index ( $\pm$ ): 1

Peaklist of GC/MS Data:

73
147
117
190
191
148

Tolerance for Peaks ( $\pm$ ): 0.1

GC/MS Search Result

There were no results found.

First Prev Next Last | 150 Rows Displayed | Export XLS

Search | Clear

HMDB ID	Common Name	Derivatized Name	Retention Index	Parent Mass (Da)	Score
---------	-------------	------------------	-----------------	------------------	-------

Webmaster: Dan Tzur and Nelson Young  
Maintained by An Chi Gou

**MS/MS Search**

Perform : MS/MS Search

To query the database using spectral pattern matching, upload the MS/MS data file for the metabolite OR paste its content in the textarea box below.

MS/MS Search

Find Metabolites

m/z of Parent Ion: 174.1 (Da) [174.1 Da for Aconitic Acid]

m/z Tolerance ( $\pm$ ): 0.1 (Da)

Instrument Type: Triple\_Quad

Fragment Ion Tolerance ( $\pm$ ): 0.5 (Da)

CID Energy Level: Low Energy

Ionization Mode: Negative

MS/MS Data File:  View format for data file [Aconitic Acid in example]

OR

Content of MS/MS Data File:

```
41.400 9.926
95.030 100.000
111.118 24.412
128.847 30.000
172.851 11.912
```

m/z (Da) and relative intensities, RI, (%), delimited by a space (" ") or a tab ("\t").  
m/z and RI MUST contain a decimal.  
m/z MUST be less than m/z of the parent ion minus 10 Da.  
Example is the MS data file for Aconitic Acid (Low Energy).

Search Results:

Rank	HMDB ID	Name	Fit(%)	RFit(%)	Purity(%)	Energy Level	Data
1	HMDB00893	Suberic acid	0.98	0.46	0.71	low	Peaklist / Spectrum
2	HMDB01264	Dehydroascorbic acid	0.47	0.84	0.58	low	Peaklist / Spectrum

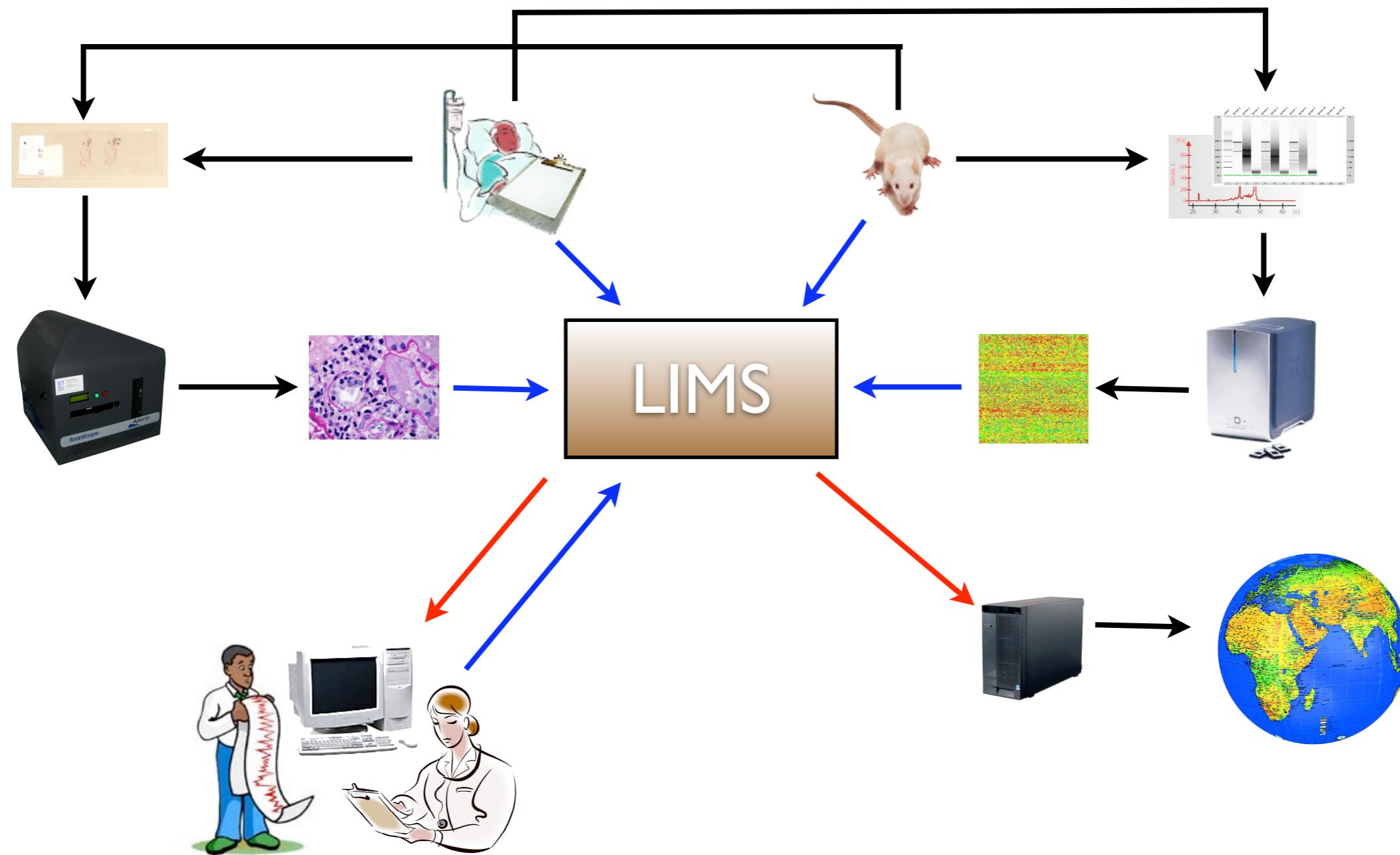
- Perform custom searches on GC/MS-MS data in the spectral databases
- Results can be filtered and searched, then exported to Excel format easily

# MetaboLIMS is Free

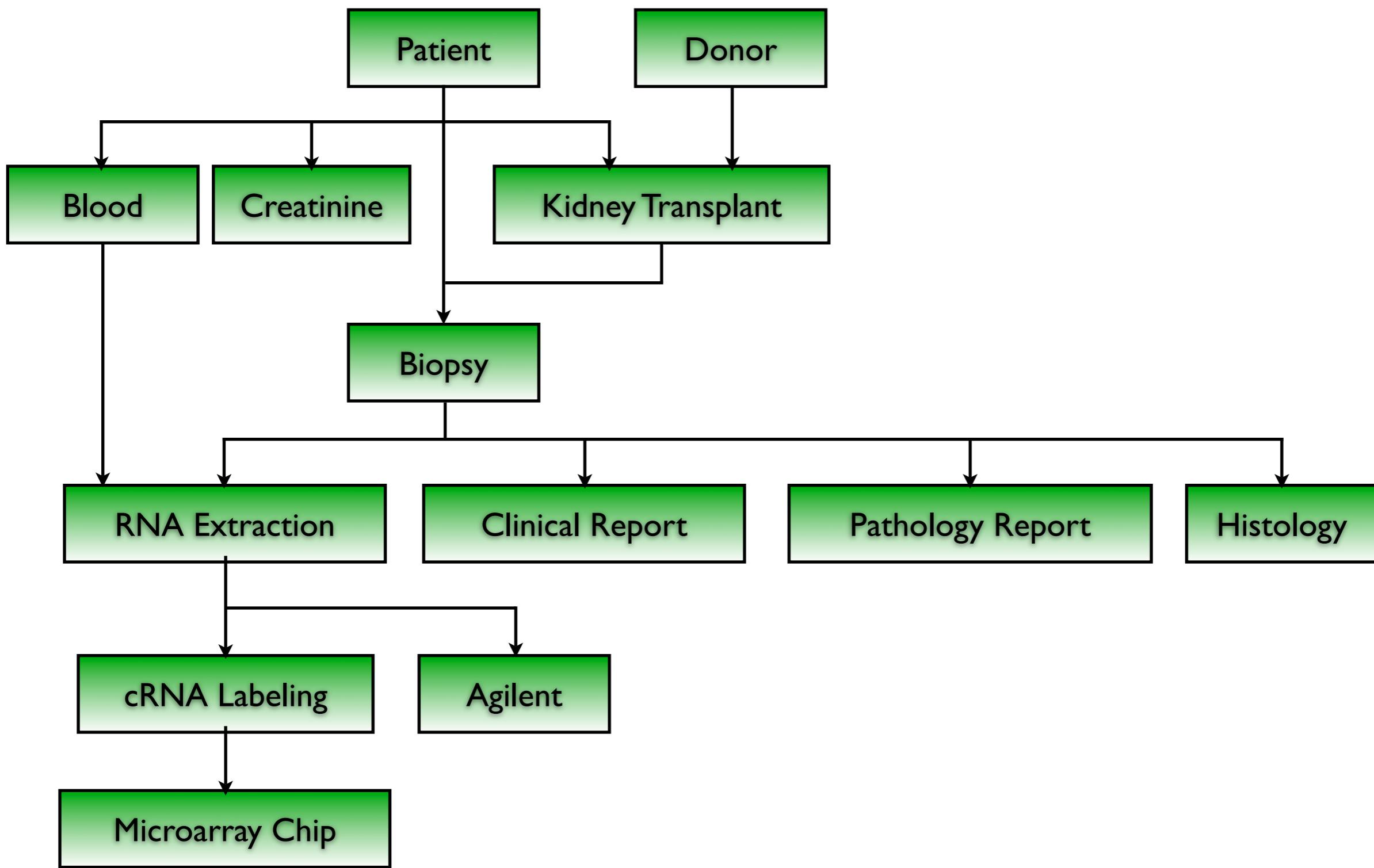
- Operational for ~12 months (lots of real-world testing)
- Still being tweaked for final release
- Trial accounts available now
- Option for HMP to host “your LIMS” or to install locally
- Installable version available for September

# **Transplant Transcriptome LIMS (Clinical LIMS)**

# Clinical LIMS



# Clinical LIMS Workflow



# Web Forms

## Pathology Report 16

[View Old Version](#)

Patient: [A-A000034](#)

Date of biopsy: [September 13, 2006](#)

Total number of glomeruli: 16

Total number of sclerosed glomeruli: 5

Diagnosis description: Persisting glomerulitis with macrophages in glomerular capillaries and prominent contours.

Comments are limited to 64 characters

Glomerulitis (g): 3

Glomerulopathy (cg): 1

Interstitial inflammation (i): 1

Interstitial fibrosis (ci): 1

Tubulitis (t): 2

Tubular atrophy (ct): 3

Intimal arteritis (v): 1

Fibrous intimal thickening (cv): 3

Arteriolar hyalinosis (ah): 0

Mesangial matrix increase (mm): 2

Peritubular capillaries (PTC) margination of inflammatory cells: 2

TCMR grade: IB

Chronic allograft nephropathy: Grade II

Electron microscopy (PTC ML) (# of layers): 4

C4D staining: Focal equivocal

BK Virus: Negative

Interstitial inflammatory cells: Macrophages

Peritubular capillaries (PTC) inflammatory cell type: Polys

Tubular necrosis: Moderate

Infarction: No

Arterial thrombosis: Mild

Venulitis: Severe

Venous thrombosis: Moderate

Edema: Moderate

Thrombotic microangiopathy: No

Casts:

Notes:

## Classifications (D2)

- ABMR
- ABMR (acute)
- Suspicious ABMR (chronic)
- ATN
- BK Virus
- Borderline
- CNIT (Calcineurin inhibitor toxicity)
- GN (Glomerulonephritis)
- Implant
- Implant (deceased donor)
- Implant (living donor)
- Nephrectomy
- Nephrectomy (Cortex)
- Nephrectomy (Medulla)
- Normal
- Protocol
- TAIF (Tubular atrophy and interstitial fibrosis)
- TCMR (T-cell-mediated rejection)
- Yes TCMR (acute)
- TCMR (chronic)
- TGP (Transplant glomerulopathy)
- Transplant nephrectomy
- Other:
- Other:

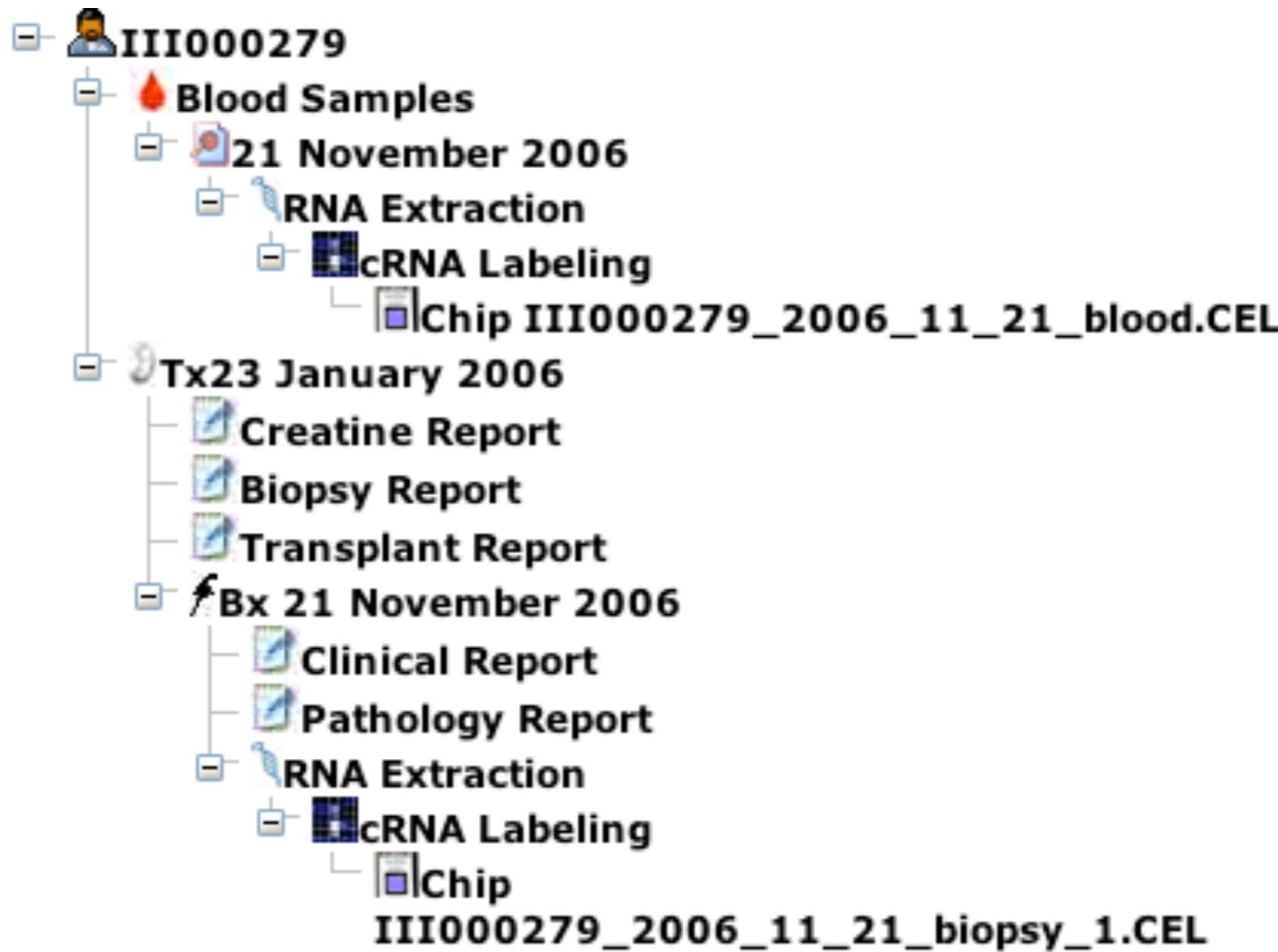
Delete

Entered by justin on 23 May 2007

Last modified by justin on 23 May 2007 13:33 MDT

[View History](#)

# Sample Tracking



- View related data for one patient

# Data Extraction

- Clinicians, statisticians, bioinformaticians, ...
- Want the data in different formats
- patient-driven? group-driven?

# Reporting

**REPORT - ATAGC TRANSCRIPTOME PROJECT**

**Disclaimer**  
Diligent efforts have been made to assure the accuracy of the information. The reporting and interpreting of data obtained from microarray measurements is novel and work in progress. Therefore, please remember, that this patient report is for information purposes only and not intended to provide clinical guidance. We disclaim all liability in connection with its use.

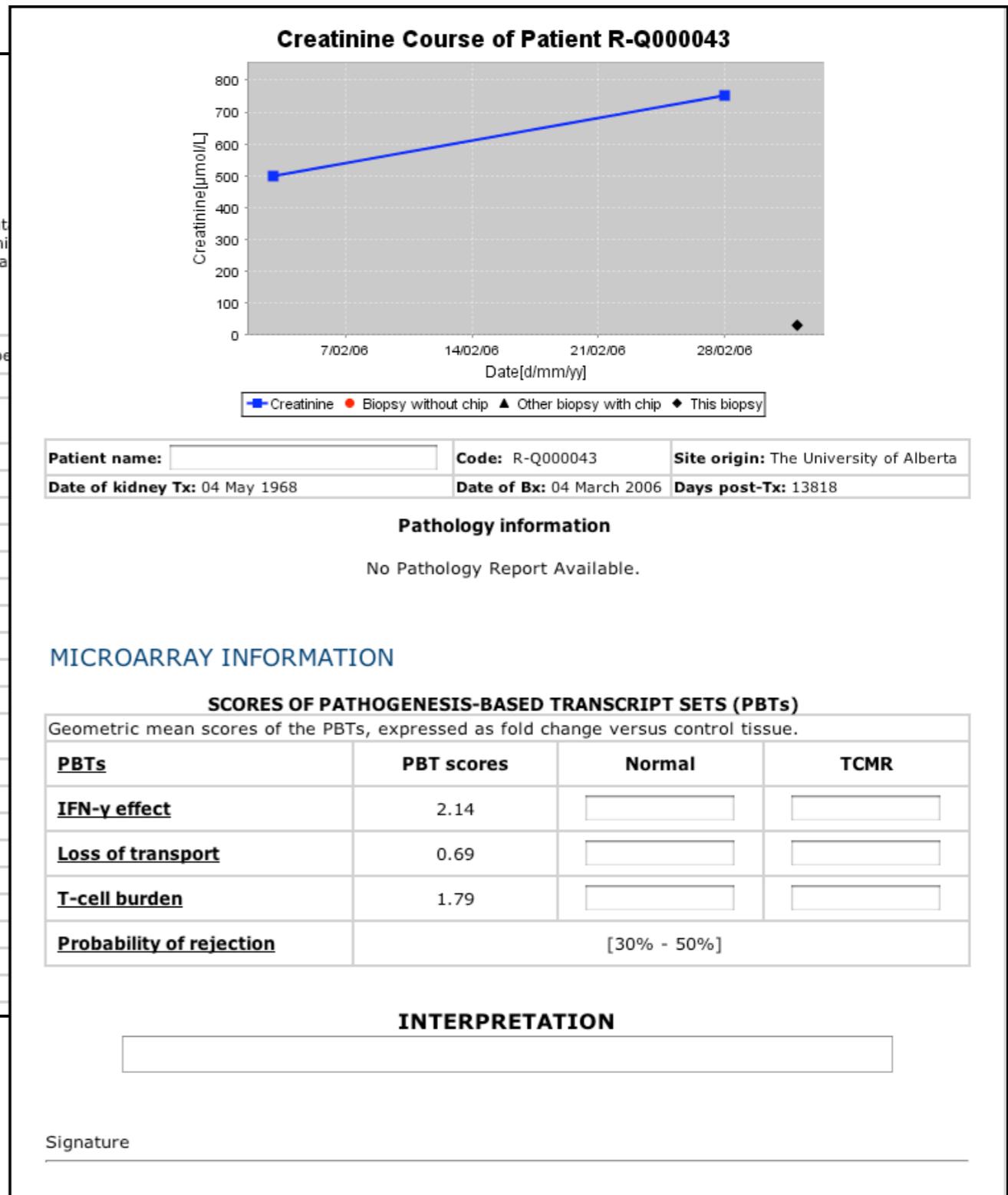
Patient name:	Code: R-Q000043	Site origin: The University of Alberta
Date of kidney Tx: 04 May 1968	Date of Bx: 04 March 2006	Days post-Tx: 13818

**Information at/around the time of transplant**

	RECIPIENT INFORMATION	DONOR INFORMATION
Type		
Gender		
Age (at time of transplant) [yrs]		
ABO		
CMV		
HLA-MM	0 T-cell (class I)	0 B-cell (class II)
PRA Peak [%]		
PRA at time of transplant [%]		

**Clinical information at/around the time of biopsy**

Indication	nephrectomy (tx)	
	1st Value	2nd Value
Hematuria(dipstick)	trace	negative
Proteinuria(dipstick)	gross	gross
Protein-to-creatinine ratio(mg/mmol)	500.0	200.0
BK Virus(P)(copies/mL)		42.0
BK Virus(U)(copies/mL)		
Maintenance immunosuppression	Cyclosporine; Everolimus	
Bolus therapy	IVIG	



# Querying

Human Query

http://192.168.20.56:8080/LIMS/LIMSServlet?cmd=setup\_human\_query

Google

Apple (99) Amazon eBay Yahoo! News (390) Slashdot (100) Shoot it!

Logged in: joey (The University of Alberta)

UNIVERSITY OF ALBERTA

Home Account Human Mouse

Clinic Wet Lab Microarray Data Lock Query Search for Genes Pre-defined Queries Customized Query Customized Query (2) Analysis

**Options**

Submit

**Display**

**Join type**

Patient

Results do not require Donor

Results do not require KidneyTransplant

Results do not require Biopsy

Results do not require Clinical Report

Results do not require Kidney Pathology

Results do not require RNA

Results do not require cRNA

Results require Chip

Display Type HTML

Kidney Pathology Filter(s)

Created by: Updated by:

Automatic:D2, D2,(collapsed), Diagnosis, Glomerulitis(g), Glomerulopathy.cg), Interstitial\_inflammation (i), Interstitial\_fibrosis (ci), Tubritis(t), Tubular\_Atrophy(ct), Intimal\_Arteritis(v), Fibrous\_Intimal\_Thickening(cv), Arteriolar\_Hyalinosis(ah), Mesangial\_Matrix\_Increase(mm), PTC\_Margination\_Of\_Inflammatory\_Cells, PTC\_ML, C4D\_staining, BK\_Virus, PTC\_Inflammatory\_Cell\_Type, CreatedBy, UpdatedBy

Number Of Glomeruli  
Number Of Sclerosed Glomeruli  
Diagnosis  
Glomerulitis  
Glomerulitis Comments  
Glomerulopathy  
Glomerulopathy Comments  
Interstitial Inflammation  
Interstitial Inflammation Comments  
Interstitial Fibrosis

Classifications (D2)

No Classification

Pending Information

Diagnosis  
PTC ML  
C4D  
BK virus

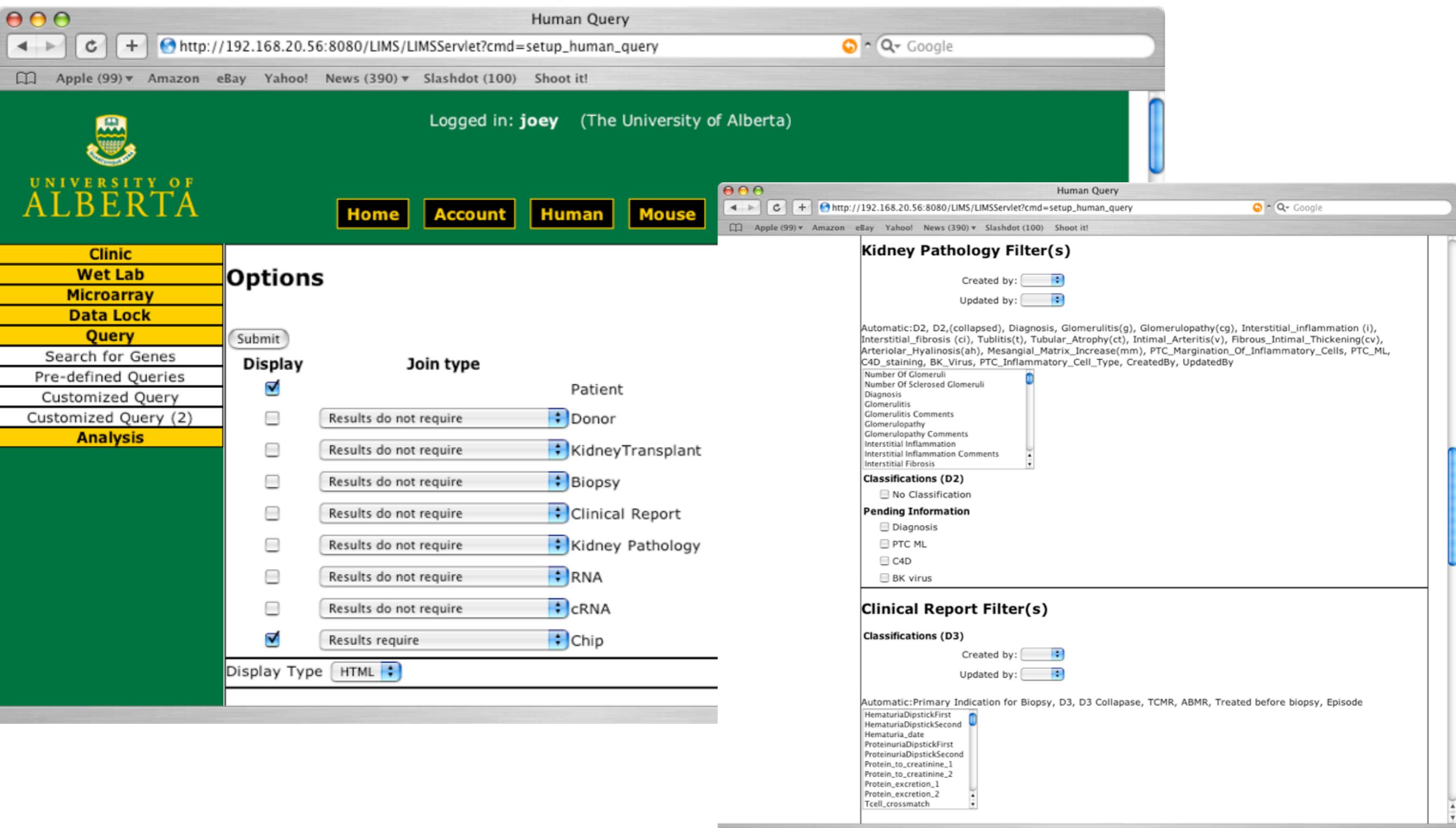
Clinical Report Filter(s)

Classifications (D3)

Created by: Updated by:

Automatic:Primary Indication for Biopsy, D3, D3 Collapase, TCMR, ABMR, Treated before biopsy, Episode

HematuriaDipstickFirst  
HematuriaDipstickSecond  
Hematuria\_date  
ProteinuriaDipstickFirst  
ProteinuriaDipstickSecond  
Protein\_to\_creatinine\_1  
Protein\_to\_creatinine\_2  
Protein\_excretion\_1  
Protein\_excretion\_2  
Tcell\_crossmatch



# Query Results

http://192.168.20.56:8080/LIMS/LIMSServlet

Apple (99) ▾ Amazon eBay Yahoo! News (390) ▾ Slashdot (100) Shoot it! Google

5 Results  
5 unique Chips

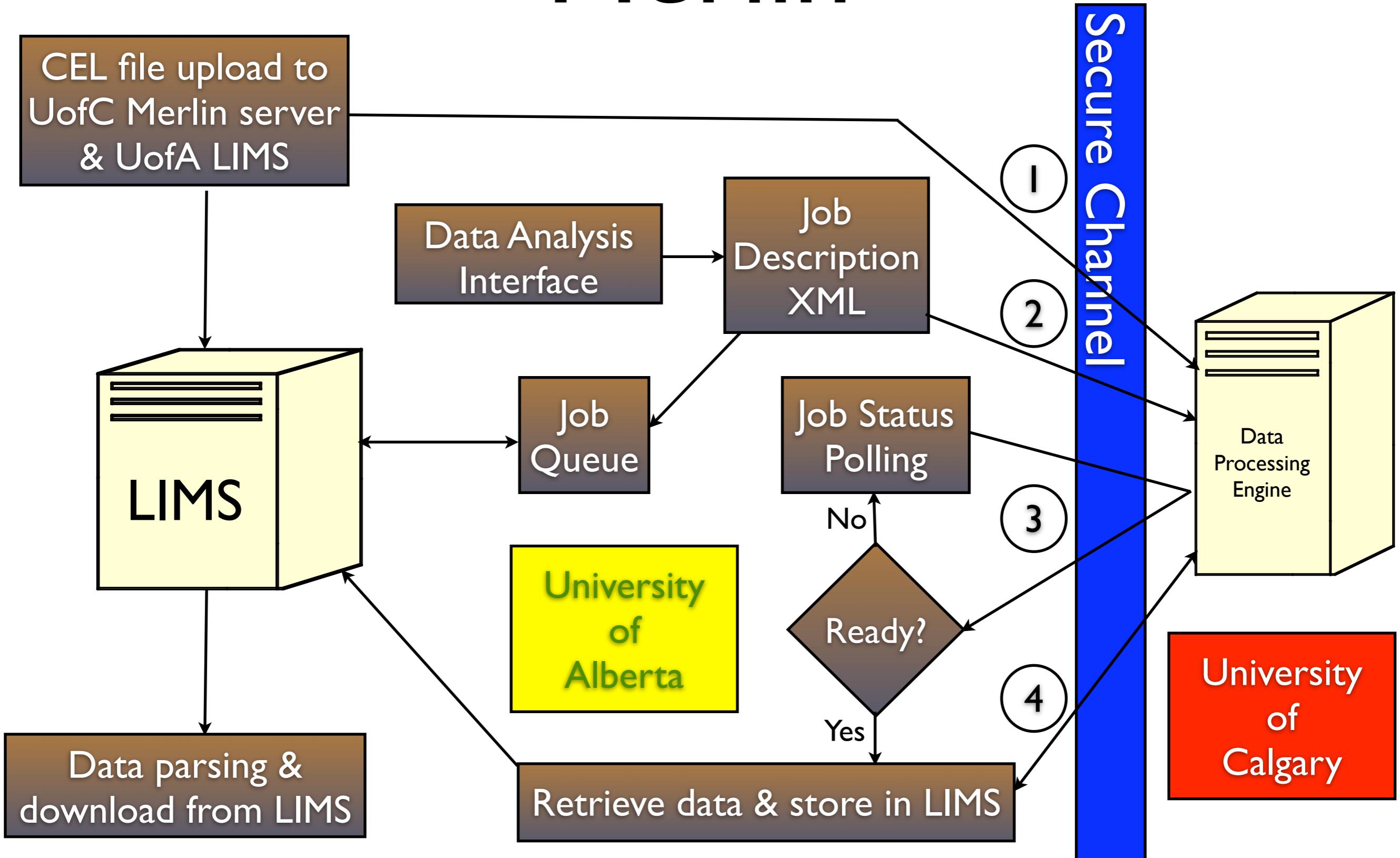
Chip		Patient		Donor		Kidney_Transplant	Other
CelFile_Name	Chip_id	Patient_ID	Patient_SiteOrigin	Donor_id	Donor_code	Date_Of_Transplant	Other
1.cel	7	34	The University of Alberta	28	DD0028	08/16/02	08/16/02
BA178_M2_2005_11_09_biopsyb_1.CEL	0	37	The Hennepin County Medical Center			04/01/06	04/01/06
ACC103-22-Aug-2005.CEL	9	32	The University of Alberta			05/04/68	05/04/68
BA178_M2_2005_11_09_biopsy_1.CEL	232	34	The University of Alberta				08/16/02
BAV96_18_May_06_biopsy_1.CEL	233	34	The University of Alberta	28	DD0028	08/16/02	08/16/02

# Common Queries

The screenshot shows a web browser window titled "Patient Listing" with the URL [http://192.168.20.56:8080/LIMS/LIMSServlet?cmd=show\\_human](http://192.168.20.56:8080/LIMS/LIMSServlet?cmd=show_human). The browser's address bar also shows a Google search bar. The page header includes the University of Alberta logo and the text "Logged in: joey (The University of Alberta)". A navigation menu at the top right includes links for Home, Account, Human, Mouse, SOP, and Logout. On the left, a sidebar menu lists Clinic, Wet Lab, Microarray, Data Lock, Query, and Analysis options. The main content area is titled "Reports" and contains a bulleted list of links:

- [Pending Kidney Pathology](#)
- [Chips with no corresponding Kidney Pathology](#)
- [Patients without any kidney transplants](#)
- [Kidney transplants without any biopsy information](#)
- [Clinical and pathology reports for all biopsies on which microarrays have been run.](#)
- [Patients with biopsies but no tested creatinine data.](#)
- [Biopsy that matches to blood samples](#)
- [New & updated Clinical and Pathology Reports, Patients, Biopsies, and Blood Samples](#)

# Merlin



# Merlin

Choose Filters - Windows Internet Explorer  
http://localhost:8080/LIMS/LIMSServlet?cmd=forwardcmd&action=submit-experiments

UNIVERSITY OF ALBERTA Microarray Data Analysis Human Chip Analysis | Mouse Chip Analysis | Use Me | LIMS | Show Merlin Jobs | Logout

Step 5/6: Choose Filters

**Analysis**

**Notes:**

- If you don't choose any filter from
- The percent of samples: if a gene

at least the specified percent of experimental samples in order to be included in the result.

- If you don't fill in the percent of samples, 0% will be used if the Min and Max are specified. That means, the gene be included as long as there is one experimental sample satisfy the filter.
- If you specify more than one filter, all the filters will be used together to filter out genes that don't satisfy any of the filters.

Fold-Change: MIN MAX % of samples (0-100)

Expression Level: t-Test p-Value (0-1): Variance : IQR

Gene List Filters (notes: some gene list may need up to 1 minute to initialize):

select all	Gene List Name	Update Time
<input type="checkbox"/>	PR_hmRT_23Nov06:	2007-02-08 16:46:12.845
<input type="checkbox"/>	PR_hmCMATcr_23Nov06:	2006-12-15 15:03:40.839
<input type="checkbox"/>	PR_hmtGRITcr_23Nov06:	2007-02-08 16:42:58.16
<input type="checkbox"/>	PR_hCATR_23Nov06:	2006-12-15 15:01:22.708
<input type="checkbox"/>	Humanized mouse CATs Feb 13:	2007-02-08 16:40:25.579
<input type="checkbox"/>	CDB:	2006-05-03 14:48:46.731

**Results**

<i>id</i>	<i>exp.mean.vctl.mean</i>	...	<i>C79.CEL.slide:ctl_mean</i>	<i>SJ94 7-June-05.CEL.slide:ctl_mean</i>
Humanized CISTs.ci.min	0.86	...	1.04	0.80
Humanized CISTs.ci.max	1.23	...	1.29	1.07
Humanized CISTs.min.name	235086_at	...	202581_at	204748_at
Humanized CISTs.min	0.39	...	0.76	0.41
Humanized CISTs.median	1.00	...	1.11	0.87
Humanized CISTs.max	3.57	...	3.86	2.60
Humanized CISTs.max.name	204438_at	...	227140_at	204438_at
Humanized CISTs.mean	1.03	...	1.16	0.93
Humanized CISTs.sd		..35		1.54
211122_s_at		.28		66.66
210163_at	23.73	...	1.35	41.91
231628_s_at	18.54	...	0.92	8.96
204533_at	18.29	...	1.76	16.9

# Patient Report

Patient name:		Code: A-A000001	Site origin: The University of Alberta
Date of kidney Tx:	01 February 1998	Date of Bx:	01 February 2000 Days post-Tx: 730

## Pathology information

Banff classification	g1, cg2, i3, ci1, t2, ct3, v1, cv1, ah2, mm3 C4d not done
Diagnosis	

## MICROARRAY INFORMATION

### SCORES OF PATHOGENESIS-BASED TRANSCRIPT SETS (PBTs)

Geometric mean scores of the PBTs, expressed as fold change versus control tissue.			
PBTs	PBT scores	Normal	TCMR
<u>IFN-<math>\gamma</math> effect</u>	0.85		
<u>Loss of transport</u>	1.05		
<u>T-cell burden</u>	0.95		
<u>Probability of rejection</u>		[0% - 10%]	

## INTERPRETATION

# GeneSpring

**Gene List Scores**

Sample	Biological Process
YW79_2005_05_29_biopsy_1.CEL.txt	0.995187601968889
YW79_2005_05_29_biopsy_1.CEL.txt	1.0045633056154497
ZPA000083_2005_06_04_biopsy_1.txt	1.0031098770810638
ZPA000083_2005_06_04_biopsy_1.txt	1.0125946542477287

**Gene List Scores**

Sex	Biological Process
female	60.103332058137234
male	60.57802377120297

**Run Script Gene List Scores**

**Inputs**

- Gene Lists/Simplified Gene Ontology/Biological Process

**Sample**

- Affymetrix/HG\_U133\_Plus\_2/Samples/ZPA000083\_2005\_06\_04.bcl
- Affymetrix/HG\_U133\_Plus\_2/Samples/ZPA000083\_2005\_06\_04.bcl
- Affymetrix/HG\_U133\_Plus\_2/Samples/YW79\_2005\_05\_29\_biopsy\_1
- Affymetrix/HG\_U133\_Plus\_2/Samples/YW79\_2005\_05\_29\_biopsy\_1

**Knobs**

(this script has no knobs)

**Notes**

(this script has no notes)

**Computation Preferences**

Compute locally    Compute on a RemoteServer

Progress: Local run time estimate: Seconds

Show: All Data

Start Close View Script Edit Script

**Import Data: Define File Format and Genome**

**File Format**

Choose File Format: Merlin

**Genome**

Select the genome (set of genes on the array) for this data. If your genome does not appear on the list, you can create a new one by selecting Create a New Genome.

**Select Genome**

**Genomes or Arrays**

**Affymetrix**

- HG\_U133\_Plus\_2
- MOE430A
- Mouse430\_2

**Demo Chips**

- Demo Human
- Demo Rat
- Yeast

**Create a New Genome**

Choose a Name:

Next... Cancel Help