

# ***PiMS, xtalPiMS and beyond: proteins, crystals and data***

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...and the PiMS development team

# Outline of talk

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- What is information management?
- PiMS concepts
- Use of PiMS for real projects
- xtalPiMS for crystallization
- Getting information to the synchrotron



# What is information management?

- **The process of storing experimental information for later retrieval**
  - Storage medium can be human memory, paper, electronic files or relational databases
  - Quality assurance (QA) experiments are typically repetitive, research experiments are constantly changing
  - Purpose of retrieval could be supporting the next experiment, providing reports, publishing papers or depositing public data
  - Automated systems may require electronic information management



# Research laboratory processes

- **Full projects (solving a protein structure?)**
  - Long workflow with many decision points
  - No two projects are identical
  - Comprise different experimental steps...
- **Routine experiments (purification, QA?)**
  - Performed the same way for several projects
- **High-throughput experiments (cloning?)**
  - Routine experiments using robots
  - Tracking of samples is paramount
- **One-off experiments (functional assays?)**
  - Unique to a particular project



# Systems for managing information

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## ■ Paper-based records

- Well suited to independent research
- Long-term archive for independent researcher

## ■ Electronic Laboratory Notebooks (ELNs)

- Electronic version of paper systems
- Can be shared remotely

## ■ Laboratory Information Management Systems (LIMS)

- Based on a relational database
- Requires a model for laboratory processes
- Snapshot of current state of laboratory



# Benefits of LIMS

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## ■ **Standardization**

- Use of controlled vocabulary and standards
- Comparing different experiments
- Depositing data in standardized form

## ■ **Distributed and collaborative processes**

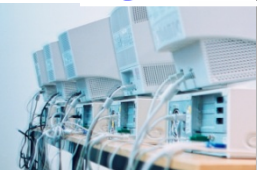
- Information can be accessed anywhere
- Different people record into same store

## ■ **Miniaturized processes**

- Labelling of samples becomes impossible

## ■ **Automated and high-throughput processes**

- Handling layouts in plates *etc.*





# Potential problems with LIMS

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## ■ IT overhead

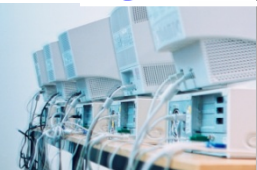
- Shared data should be on backed-up server – use a web-based service

## ■ Data loss

- Hardware failure or data corruption – hardware failures manageable

## ■ Data integrity

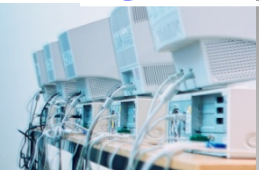
- Data need to be entered properly or LIMS can default to being ELN
- Recording data takes time for no immediate benefit – easy input essential
- Unrecorded data are lost and incomplete data may break data “chain”





# What is PiMS?

- **Protein Information Management System**
  - Collaborative academic effort to produce a general free-to-use fully featured LIMS
- **PiMS needs to support anyone & everyone**
  - Data for complex ever-changing workflows
  - Data need to be recorded in standardized ways
  - Many labs have similar processes
  - Most have some unique processes
- **PiMS needs to be very easy to use**
  - Schema reflects workflow: specific to one site, specific to one workflow, hard to modify
  - Schema generalizes samples and processes: flexible but potentially hard to use







# Technologies used in PiMS

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## ■ PiMS is a web application

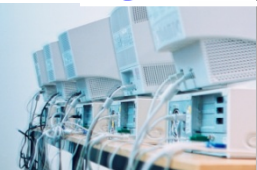
- Client is Mozilla Firefox or Internet Explorer
- No client software to install (perhaps plugins)
- Windows, Macintosh and Linux clients

## ■ PiMS requires a server – or two

- Web server uses Apache Tomcat
- Database server uses PostgreSQL or Oracle
- Windows and Linux servers
- Managed public PiMS server hosted at RAL

## ■ Technologies used by developers

- Java1.5, Hibernate, JUnit, BioJava, dot, batik, AJAX, ...





# PiMS uses simple key concepts

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## ■ Complexes & Targets

- Descriptions of proteins and complexes
- Can contain bioinformatics annotations

## ■ Constructs

- Starting point for real experiments
- Describes actual sequences

## ■ (Typed) Samples

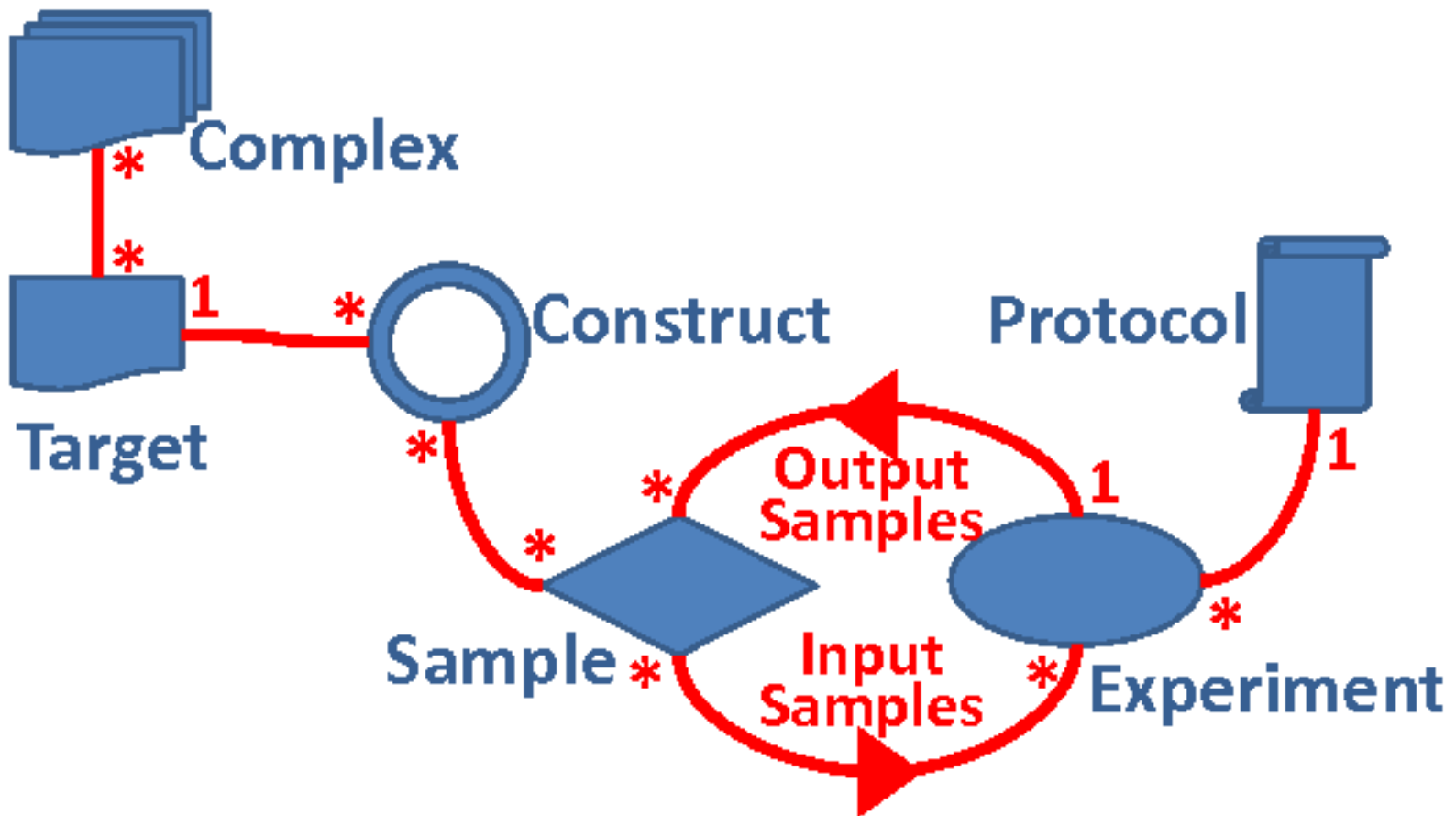
- Tracked samples made & used by experiments
- Samples have types, owners, locations *etc.*

## ■ Experiments & Protocols

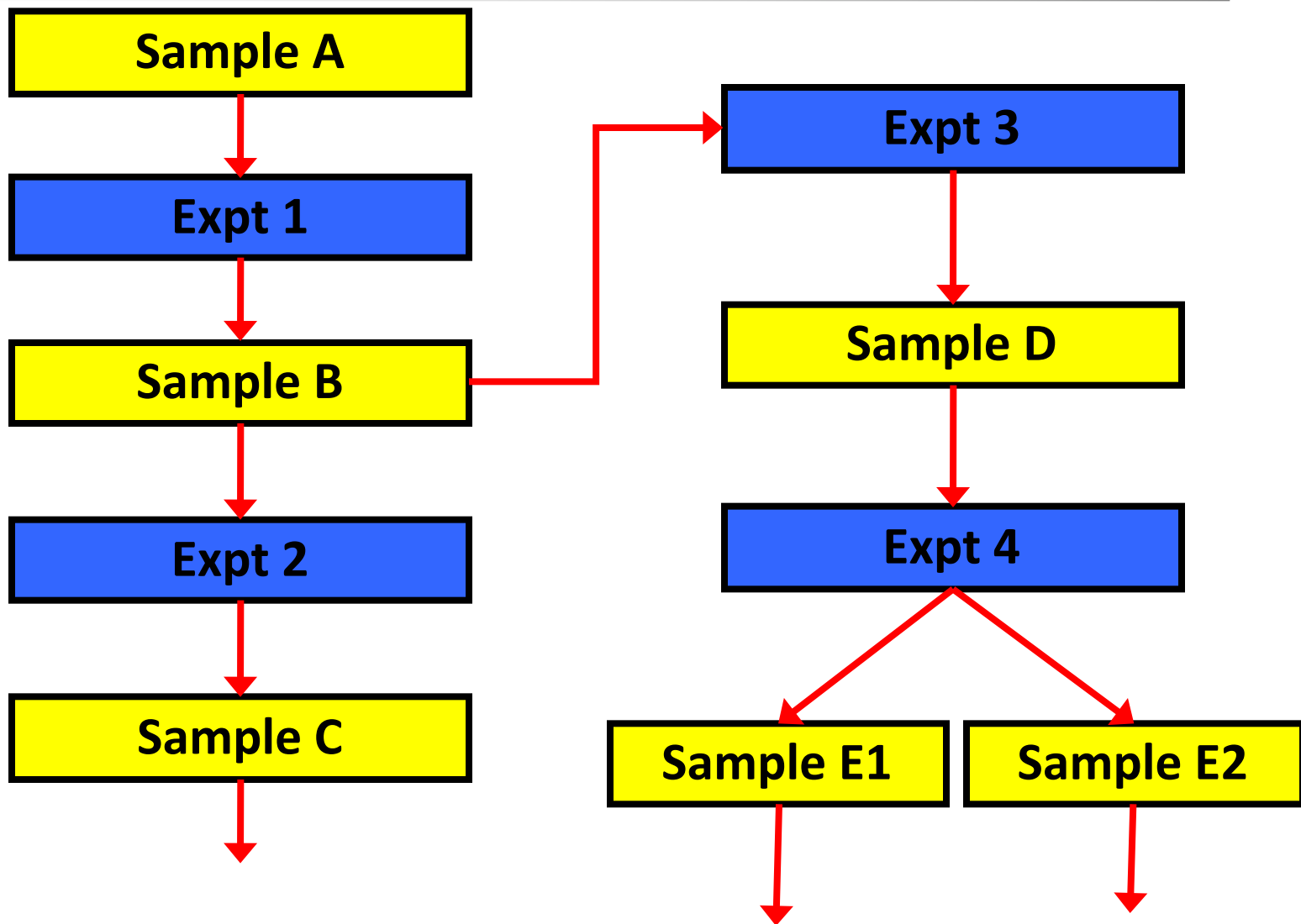
- Consume (input) and produce (output) samples
- Protocols are user-defined reusable templates



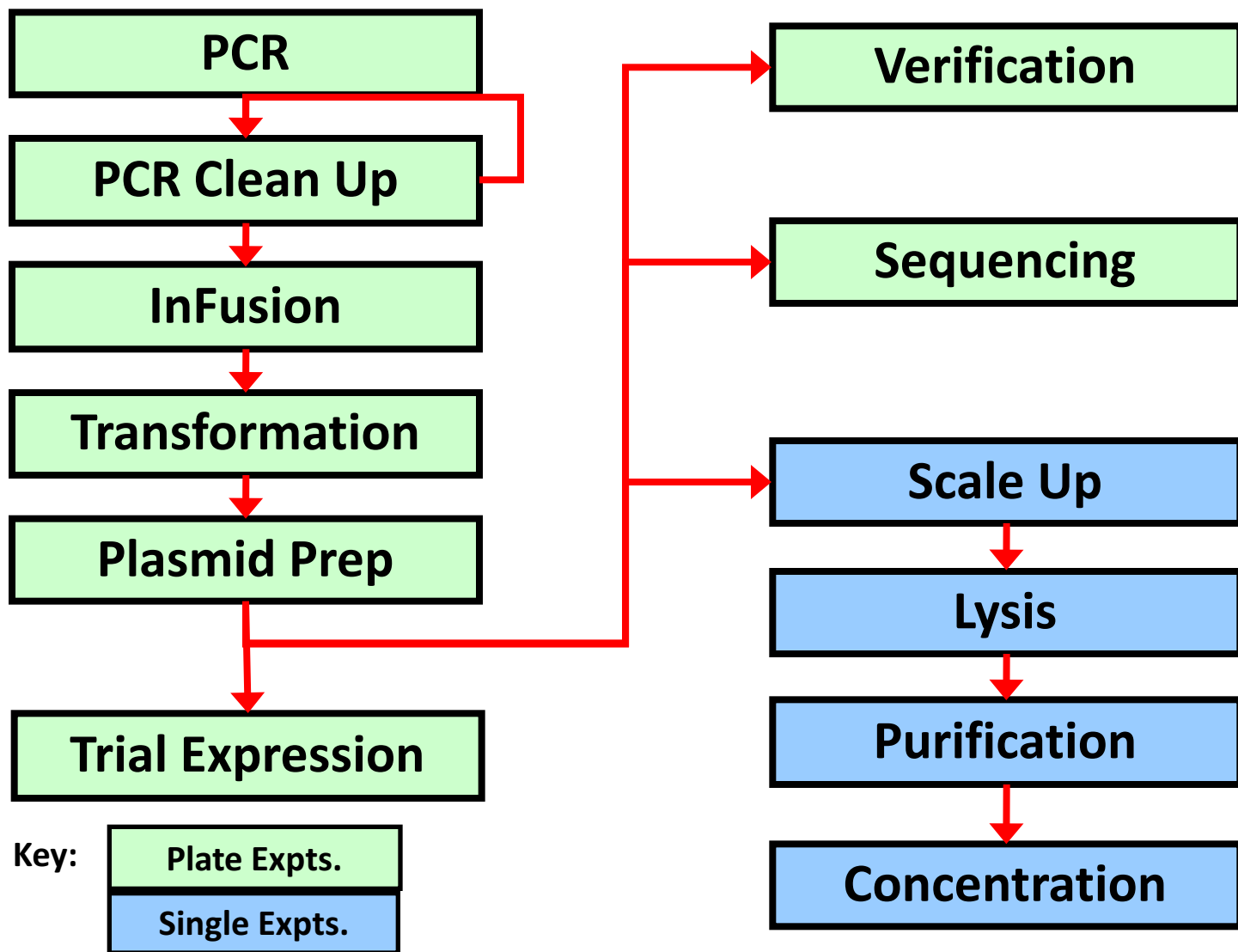
# How it all links together



# Experiments + Samples = Workflows



# Basic protocols used at OPPF



# The PiMS (v3.1) home page

**PiMS 3.1 - Mozilla Firefox**

File Edit View History Bookmarks Tools Help

http://www.oppf.ox.ac.uk/pims/

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Home Log out administrator Target OPPF Experiment Sample User History Help Perspective: OPPF

### Calendar

Click on a day to view activity on that day.  
Or view [today's activity](#).

Jun 2009

S	M	T	W	T	F	S
	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30				

### Create a new target

**Download target details:**

Enter the Database ID  
Select a database from the list  
Click "Get record"

**Database ID**

**Database**

### History

Recently viewed items

- PCR137\_PCR2\_XTREME ▼
- mShh-hHippdeltaN ▼

### Constructs no progress for 7 days

[Full Report](#)

None

### Active targets (any user)

**All Active Targets**

- OPTIC12198 ▼
- OPTIC12224 ▼
- OPTIC12225 ▼
- OPTIC12207 ▼
- OPTIC12190 ▼
- OPTIC12209 ▼
- OPTIC12217 ▼
- OPTIC12199 ▼
- OPTIC12222 ▼

### Target management

- [Sequence similarity search](#)
- [Record a new target](#)
- [Search targets](#)
- [Construct and target reports](#)

### Experiment management

- [Search experiments](#)
- [Search protocols](#)
- [Record a new experiment](#)
- [Record a new plate experiment](#)

### Search holders by barcode

### Leads Construct

Construct

**Shows recent activity and gives quick links to common steps**

**PiMS** Protein Information Management System  
Version 3.1

Done



# Standardized PiMS pages

Sample/Stock: 1232536270348 Plasmid - Mozilla Firefox


File Edit View History Bookmarks Tools Help




http://www.oppf.ox.ac.uk/pims/View/org.pimslims.model.sample.Sample:361786

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Home Log out administrator Target OPPF Experiment Sample User History Help

Perspective: OPPF

 Samples : **70348 Plasmid**


 [Diagram](#)  [Target to Crystal Report](#)  [Delete](#) Can't divide sample - set an amount first.

**Details**

Name*	1232536270348 Plasmid	Stock available	<input checked="" type="radio"/> Yes
Amount	21.0		<input type="radio"/> No
	uL	Location	No location recorded for this sample <a href="#">Set sample location</a>
Details		Use by date	
		Assigned to	none
		(Cancel editing)	

**Extra details**

**Recipe** None

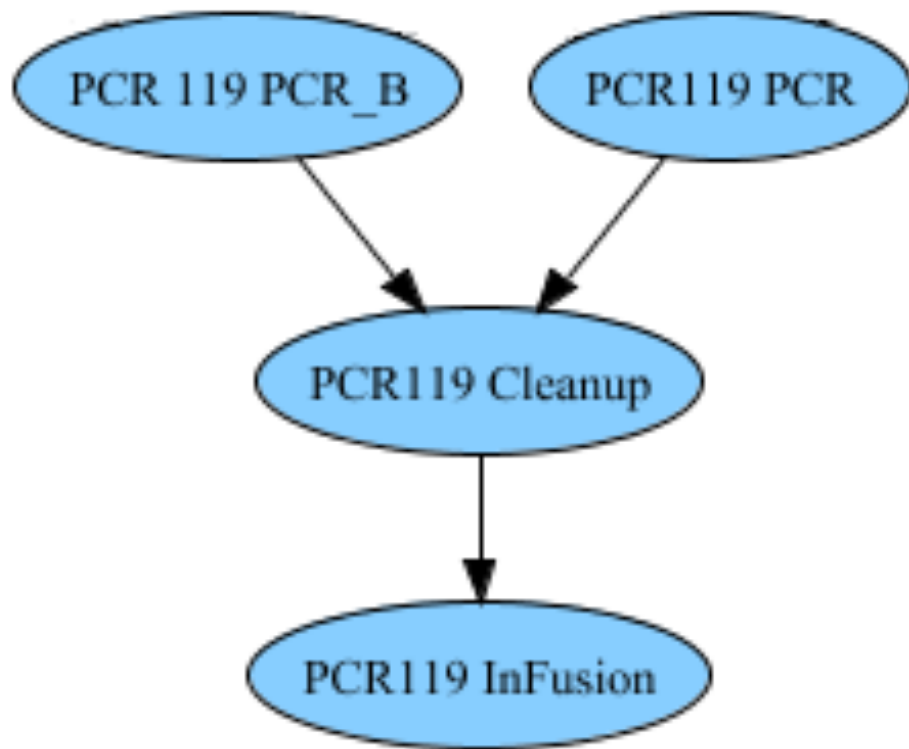
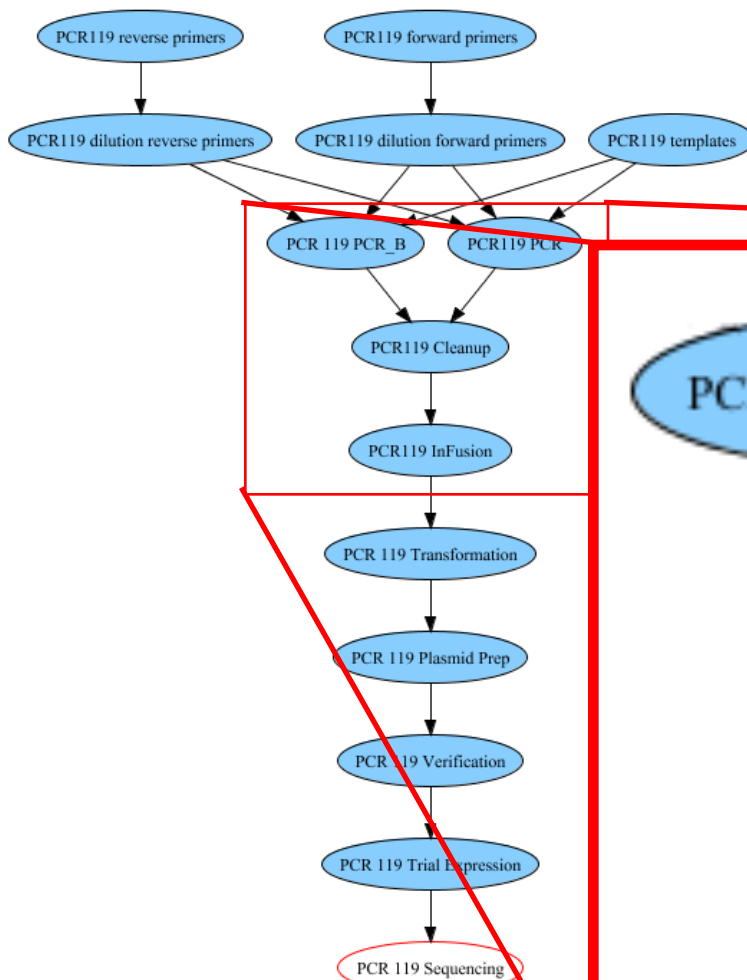
**Output Sample from Experiment:**  Ligation 2 ▼

Parameter	Value
Notes	
Total Volume (uL)*	21

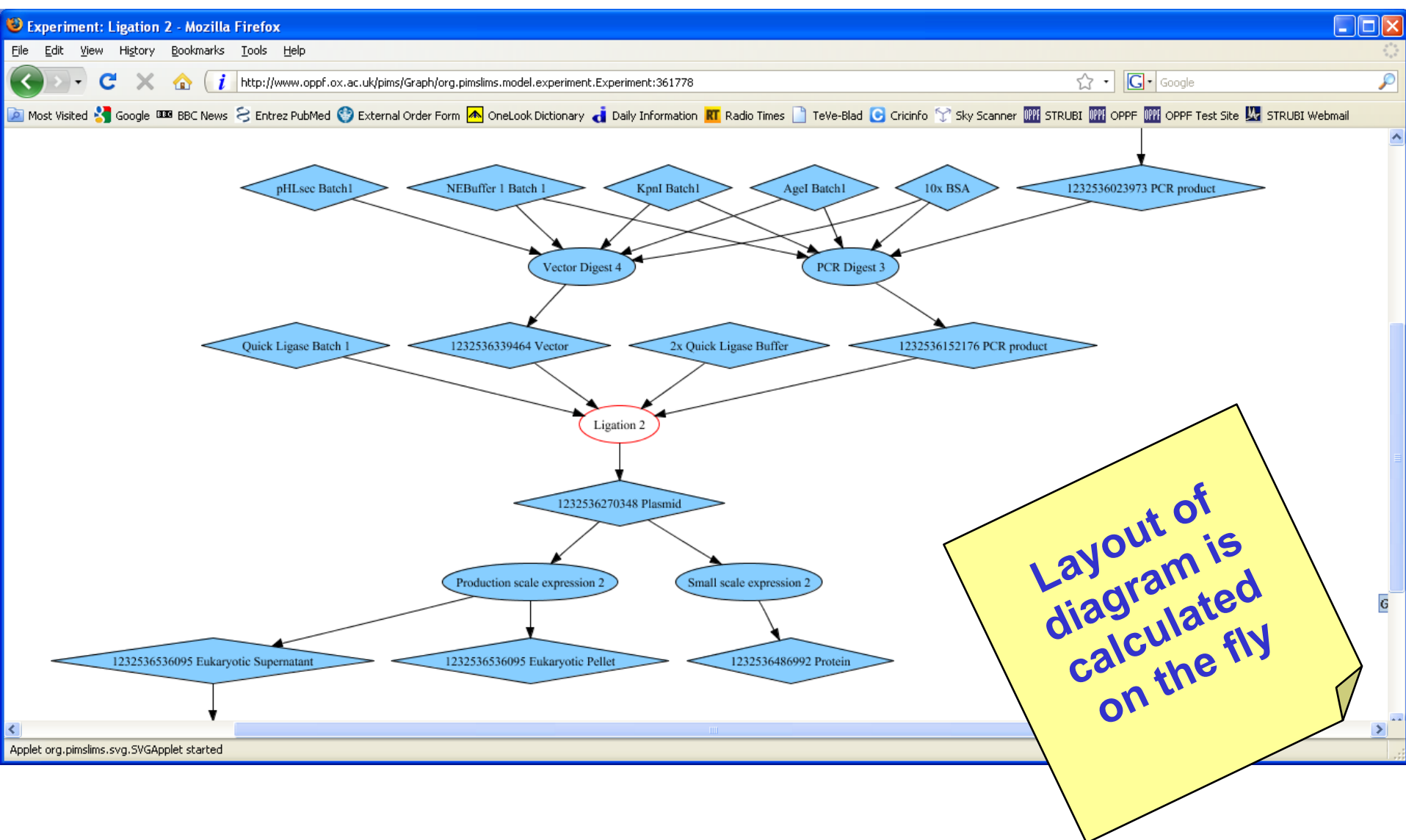
Done

**Consistent screen layout for samples, experiments & protocols**

# Navigating through your PiMS data: interactive diagrams



# Example of a complex workflow



# Experiments can read/write data



OperonOrderFormPCR119Or29917  
Microsoft Excel Worksheet  
47 KB

Microsoft Excel - OperonOrderFormPCR119Or29917

File Edit View Insert Format Tools Data Window Help

A1 CUSTOMER CONTACT, SHIPPING + INVOICE DETAILS

et	OPPF	Experiment	People &
Ac	OPPF Functions	Import from Optic	
	Primer Order Form		
	Primer Order Form Help		

A	B	C
CUSTOMER CONTACT, SHIPPING + INVOICE DETAILS		
Details	Ship to	Bill To
Name	Ray Owens	Finance Department
University/Company	Wellcome Trust Centre for Human	Wellcome Trust Centre for Human
Department	OPPF	Accounts Division
Street	Roosevelt Drive	Roosevelt Drive
City	Oxford	Oxford
Post code	OX3 7BN	OX3 7BN
	UK	UK
tel. No.	01865 287500	01865 287500
email:	ray@strubi.ox.ac.uk	ray@strubi.ox.ac.uk

Export options: CSV | Excel

1	OLIGO ID	SEQUENCE
2	OPPF3926F	AAGTTCTGTTTCAGGGCCCCGaaacagaagagtgttttcaaggatataaccagg
3	OPPF4861F	AAGTTCTGTTTCAGGGCCCCGgaaacagcatgaaatccacccc
4	OPPF4864F	AAGTTCTGTTTCAGGGCCCCGccagagtttaccatggctgctg
5	OPPF4184F	AAGTTCTGTTTCAGGGCCCCGaagaagcaccacaagccccactg
6	OPPF4867F	AAGTTCTGTTTCAGGGCCCCGagcagccacctggaggactacagt
7	OPPF4870F	AAGTTCTGTTTCAGGGCCCCGggcctgtgcttcacctttgg
8	OPPF4873F	AAGTTCTGTTTCAGGGCCCCGaccctgcggtgccttgagcc
9	OPPF4876F	AAGTTCTGTTTCAGGGCCCCGaaggaaacatttaccctggtaaatacattacctttgg
10	OPPF4879F	AAGTTCTGTTTCAGGGCCCCGctggagacagccataccatgtagc

Order details nr.5 / plate1 / plate2 / plate3 /

# Simple reports of how samples are made

- Construct: OPPF3952
- Experiment: ExperimentOPPF3952
- Experiment: PCR107 PCR:E10
- Experiment: PCR107 InFusion:E10
- Experiment: PCR107 Transformation:E10
- Experiment: PCR107 Plasmid Prep 1:E10

Export to PDF

Export to Spine2

## Experiment: ExperimentOPPF3952

### Details

### Input Samples

### Parameters

Forward Primer Tm : -1.0

Reverse Overlap : 22

Forward Overlap : 31

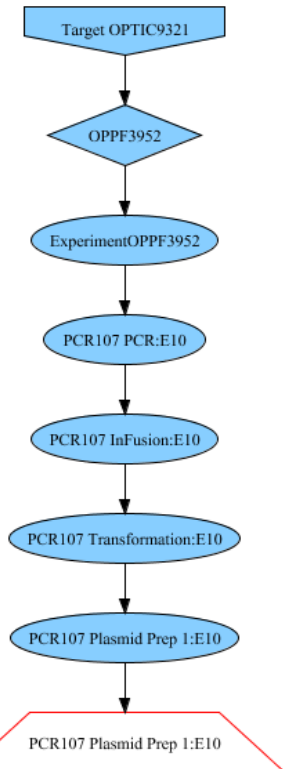
Reverse Primer : ATGGTCTAGAAAGCTT

Forward Primer : AAGTTCTGTTTCAGGGC

Reverse Primer Tm : -1.0

Forward Tag : Opti3Clnffwd

Reverse Tag : Infusion 3' site



# Graphical interface for plate experiments

Plate PCR119 Cleanup, well A1
















Target OPPF3926








Kit: 90.0uL, **Unspecified**

PCR product: 50.0uL PCR119 PCR:A01

Checked on gel?: Yes

Status: To be run

												
	1	2	3	4	5	6	7	8	9	10	11	12
 A												
 B												
 C												

Basic details		Quick setup		Plate view	Spreadsheet view	Files	
Tray	Row	Col	Target	Status	Output	Kit	
						Sample	Vol uL
PCR119 Cleanup	A	1	OPPF3926	To be run 	PCR119 Cleanup:A01	(None)	90.0
PCR119 Cleanup	B	1	OPPF4861	To be run 	PCR119 Cleanup:B01	(None)	90.0
PCR119 Cleanup	C	1	OPPF4864	To be run 	PCR119 Cleanup:C01	(None)	90.0
PCR119 Cleanup	D	1	OPPF4184	To be run 	PCR119 Cleanup:D01	(None)	90.0
PCR119 Cleanup	E	1	OPPF4867	To be run 	PCR119 Cleanup:E01	(None)	90.0
PCR119 Cleanup	F	1	OPPF4870	To be run 	PCR119 Cleanup:F01	(None)	90.0
PCR119 Cleanup	G	1	OPPF4873	To be run 	PCR119 Cleanup:G01	(None)	90.0

Interface being reworked for next release of PiMS



# The xtalPiMS home page

[xtalPiMS] : Home - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://www.opf.ox.ac.uk/xtalpims/Home.jsp

Most Visited Google BBC News Entrez PubMed External Order Form OneLook Dictionary Daily Information RT Radio Times TeVe-Blad Cricinfo Sky Scanner STRUBI OPPE OPPF STRUBI Webmail

## xtalPiMS

Home Logout: robert View Screens Help

### Recent Plate Inspection Summary

1 2 3 4 5 ... 206

Date	Barcode	Imaging System
07/01/2010 08:08	441300363516	Oasis 1700 (20.5°C)
07/01/2010 08:07	441300363554	Oasis 1700 (20.5°C)
07/01/2010 08:06	441300363530	Oasis 1700 (20.5°C)
07/01/2010 08:05	441300363684	Oasis 1700 (20.5°C)

### Most Recent Annotations

1 2 3 4 5 ... 15

Barcode	Well	Date	Description	Annotator	Version	Type	Inspection
441300313085	C05.1	06/01/2010 17:06	Potential Crystals	Shuo	-	human	-
441300297064	E04.1	06/01/2010 13:23	Crystals	dimattia	-	human	-
441300303567	F01.1	05/01/2010 19:20	Salt Crystals	dan	-	human	-
441300303567	E10.1	05/01/2010 19:20	Salt Crystals	dan	-	human	-

### Recent Microscope Images

441300315836-B05.1 441300315829-B02.1 441300362984-H04.1 441300362984-H04.1

### My Groups

1 2 3 4 5 ... 78

Name	Group Head	
Adenovirus IVa2	erika	Unkn
Aeropath	ray	Unkn
AIV	dave	Unkn
AMPA	radu	Unkn

Boxes show latest updates for projects that you have access to

Done

FileEditViewHistoryBookmarksToolsHelp

<>CXX

talhttp://www.oppf.ox.ac.uk/xtalpims/ViewTrialDrops.jsp?barcode=441300356020&name=441300356020-20080814-19

Google

Most VisitedGoogleBBCBBC NewsEntrez PubMedExternal Order FormOneLook DictionaryDaily InformationRTRadio TimesTeVe-BladCricinfoSky Scanner

HomeLogout: robertViewScreensHelp

Navigation - plate 441300356020

K<<>>L

Delay: - 0.2 +

	1	2	3	4	5	6	7	8	9	10	11	12
A												
B												
C												
D												
E												
F												
G												
H												

Information - well C01.1

16/5/2009walterCrystals

ATAD2 BROMODOMAIN#3 C-terminal HisTagged - SeMet, 9 mg/ml + DTT - Additive screen 96-well Hampton

Taken at: Thu, 14 Aug 2008 18:46:17 GMT

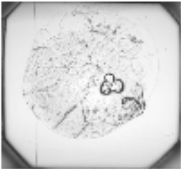
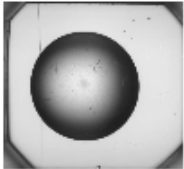
Taken by: Oasis 1700 (20.5°C)

Screen:

Condition: Unspecified

[View Microscope Images](#)

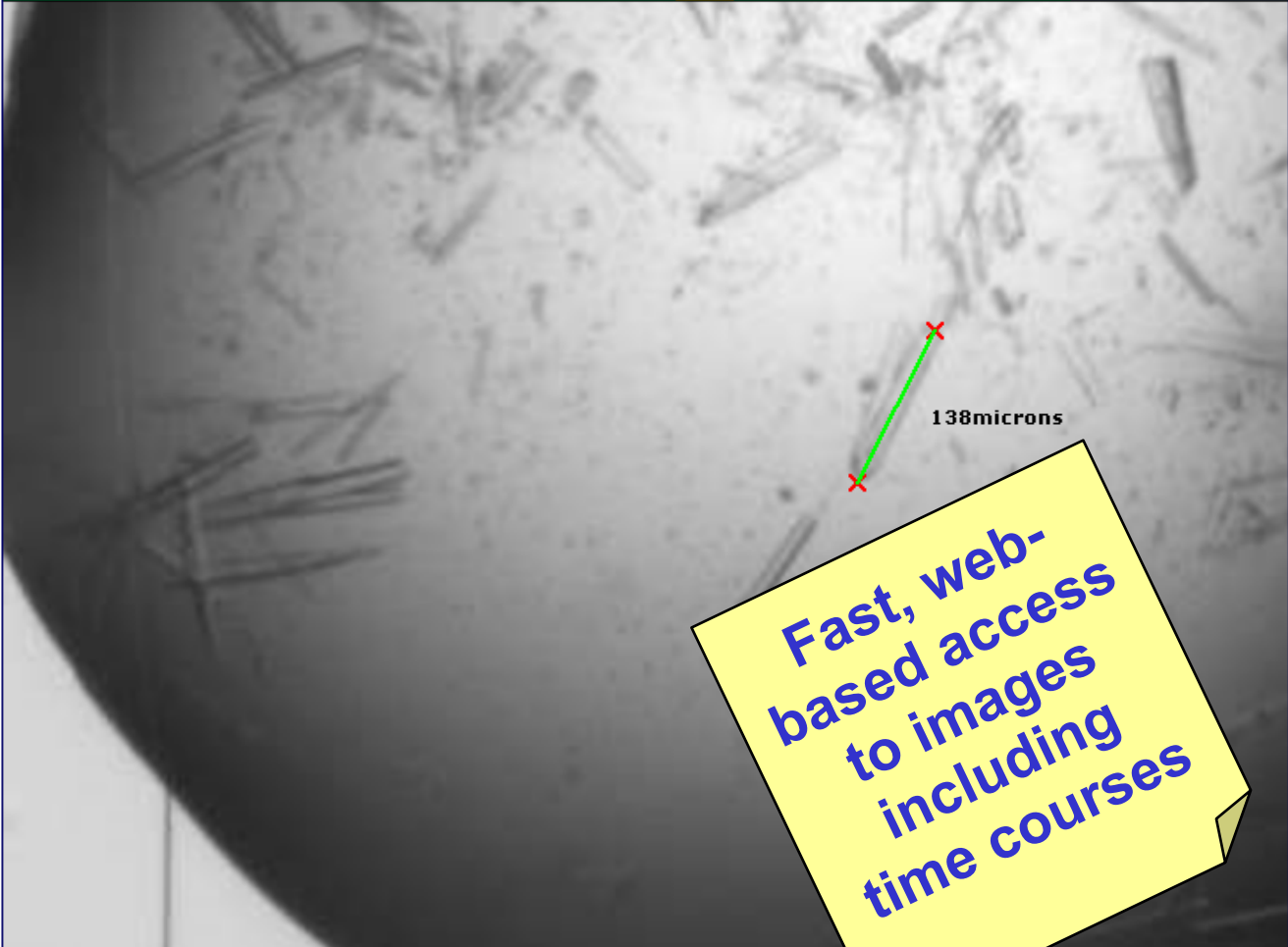
EarliestLatest



[Full time course...](#)

441300356020-C01.1 +8 days 01:07:16

PIXZoom: 200%Annotate:



Fast, web-based access to images including time courses

Done

[xtalPIMS] : View Trial Drops - Mozilla Firefox

File Edit View History Bookmarks Tools Help

tal http://www.oppf.ox.ac.uk/xtalpims/ViewTrialDrops.jsp?barcode=441300356020&name=441300356020-20080814-19 Google

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## Help for View Trial Drops v3

Key	Function
f	Toggle navigation mode (Search list / Timecourse)
a	Go to previous image in Search list / Timecourse
d	Go to next image in Search list / Timecourse
q	Go to first image in Search list / Timecourse
e	Go to last image in Search list / Timecourse
\	Go to well F01.1 (Search list only)
s	Toggle (Start/Stop) movie
z	Zoom out
x	Reset zoom to 100%
c	Zoom in
v	Zoom to fit (also resets image position to origin)
1-9	Annotate image from Clear (0) to Synchrotron (8)

## Main Image Mouse Gestures

Gesture	Function
Ctrl+Drag	Reposition image
Drag	Measure image
DblClick	Zoom in on clicked pixel
Ctrl+DblClick	Zoom out on clicked pixel

Done

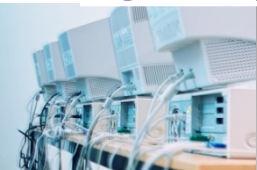
# Moving along the pipeline: linking to X-ray data collection

## ■ Changing ways of using synchrotrons

- Rapid data collection means more samples
- Expert users collect data for many projects
- Increasing use of remote access
- Ever more automation which needs data

## ■ Can PiMS and xtalPiMS help?

- Easy report of sample details from PiMS
- xtalPiMS can mark crystal for data collection
- Need simple project planning tool in xtalPiMS
- *In situ* diffraction screening plan for xtalPiMS
- eHTPX-style message model to get data to ISPyB *etc.*



# Acknowledgments

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## ■ The PiMS project people

- Kim Henrick, Dave Stuart, Keith Wilson, Colin Nave, Neil Isaacs, Jim Naismith, Richard Blake
- Chris Morris
- Ed Daniel, Alain Da Souza, Jon Diprose, Susy Griffiths, Bill Lin, Anne Pajon, Katya Pilicheva, Marc Savitsky, Petr Troshin, Jo van Niekerk

## ■ xtalPiMS (and Vault) people

- Ian Berry, Chris Mayo

## ■ PiMS and xtalPiMS users in Oxford

- Ben Bishop and Christian Siebold

