



Protein Information Management System (PIMS)

Robert Esnouf

Oxford Protein Production Facility,
University of Oxford...

...and the PIMS development team

PSDI XV 2007, Autrans, 30/10/2007



Outline of talk



- Background to PIMS
 - What is PIMS?
 - Why develop PIMS?
 - Why am I here?!?
- Basic concepts of PIMS
 - Targets and Constructs
 - Samples
 - Experiments and Protocols
 - Workflows
- PIMS at the OPPF
 - A short demonstration of tracking science
- Come and play for yourselves
 - PIMS on Oracle



What is PIMS?



- BBSRC SPoRT funded two consortia:
 - Scottish Structural Proteomics Facility (SSPF)
 - Membrane Protein Structure Initiative (MPSI)

- PIMS is funded to develop a laboratory information management system (LIMS):
 - Funded by the BBSRC SPoRT initiative
 - Funding Jan 2005 – Dec 2009
 - Supports SSPF, MPSI, OPPF & YSBL
 - Developers in Daresbury, EBI, OPPF & YSBL
 - Support from OPPF, Dundee & Daresbury

- <http://www.pims-lims.org/>



PIMS development laboratories



PIMS PIs

- Kim Henrick, Dave Stuart, Keith Wilson, Colin Nave, Jim Naismith, Neil Isaacs



PIMS supported

- Anne Pajon, Ed Daniel, Marc Savitsky, Susy Griffiths

CCP4 supported

- Chris Morris (project manager), Bill Lin



Other support

- Robert Esnouf (scientific sponsor), Jon Diprose
- Petr Troshin, (Jo van Niekerk)
- (Ian Berry, Gael Seroul, Diederick De Vries)





Why develop PIMS?



- Longstanding need for rational data management for protein production
 - Complex, ever-changing workflow
 - To exploit higher throughput
 - To aid collaboration and make data public
- Academic LIMS (and industrial?)
 - LISA, HalX, SESAME, MOLE, (Beehive)
 - Specific to one site, hard to maintain
- PIMS is a collaborative effort to find a common solution
 - Most laboratories have some similar processes
 - All have some unique processes
 - PIMS is fully featured LIMS, not target tracking



Some ancient history

- Starts with 2001 Airlie House agreement
 - To share protein production data
 - TargetDB is limited implementation
 - Detailed specification of terms
- European-based projects
 - eHTPX: data exchange models (dictionaries)
 - HAL & HALX: LIMS concentrating on workflow
 - MOLE: LIMS built on generic data model
 - SPINE encouraged collaboration
- Loose PIMS consortium formed to seek a common solution
 - BBSRC SPoRT provided funding opportunity





Technologies used



- PIMS is used from a web browser
 - Mozilla Firefox or Internet Explorer
 - No client software to install (perhaps plugins)
 - Windows, Macintosh and Linux clients
- PIMS requires a web and database server
 - Typically the same machine
 - Web server Apache Tomcat
 - Development on free PostgreSQL
 - Now available for Oracle
 - Windows and Linux servers
- Technologies used by developers
 - Java1.5, Hibernate, JUnit, BioJava, dot, batik, AJAX, ...



Why am I here?!?



- PIMS is developing rapidly
 - Many problems overcome such as scalability and performance
 - Usability being addressed
- Academic LIMS developed to commercial standards
 - Multisite development makes it suitable for many sites
 - Industrial research laboratories not that different from academic ones
- Want to assess industrial interest in PIMS
 - Consortium-type agreements to fund continued development
 - Happy to offer on-site demonstrations



Protein Information Management System 1.3

Perspective: standard

Active samples older than 7 days

- PCR 119 PCR B:H06
- PCR 119 PCR B:H04
- PCR 119 PCR B:H03
- PCR 119 PCR B:H02
- PCR 119 PCR B:H01
- PCR 119 PCR B:G06
- PCR 119 PCR B:G04
- PCR 119 PCR B:G03
- PCR 119 PCR B:G02
- PCR 119 PCR B:G01

Active samples ready for use

None

[All Samples ready for next](#)

History

A list of your most recently viewed items.

- PCR 119 Sequencing
- OPPF Primer Order Plate
- PCR119 Order
- OPTIC9304
- PCR119 Order:A1
- PCR 119 PCR B:H01
- PCR119 forward primers
- PCR119 Cleanup

Leads construct management

[Load Primer Order Construct Management](#)

(Empty)

Samples assigned to any user

- PCR 119 PCR B:H06
- PCR 119 PCR B:H05
- PCR 119 PCR B:H04
- PCR 119 PCR B:H03
- PCR 119 PCR B:H02
- PCR 119 PCR B:H01
- PCR 119 PCR B:G06
- PCR 119 PCR B:G05
- PCR 119 PCR B:G04
- PCR 119 PCR B:G03

Constructs no progress for 7 days

None

[Construct progress report](#)

Search by barcode

Search











Finding out more

For help using PiMS, please see the [Guide to using PiMS](#).

For more details on the project, visit the [PiMS web site](#).

(Empty)

Active samples older than 7 days

-  [PCR 119 PCR B:H06](#) ▼
-  [PCR 119 PCR B:H04](#) ▼
-  [PCR 119 PCR B:H03](#) ▼
-  [PCR 119 PCR B:H02](#) ▼
-  [PCR 119 PCR B:H01](#) ▼
-  [PCR 119 PCR B:G06](#) ▼
-  [PCR 119 PCR](#)
-  [PCR 119 PCR](#)
-  [PCR 119 PCR](#)
-  [PCR 119 PCR](#)

Search by barcode

30405199304

Search



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(Empty)

Protein Information Management System 4.2 - Mozilla Firefox

File Edit View History Bookmarks

Google Perspective: standard

PIMS

Home Log out administrator Ta

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Leads construct management

[Load Primer Order](#)
[Construct Management](#)

(Empty)

Search by barcode

Search

(Empty)

http://localhost:8080/pims-oracle/View/

start Protein Informat...

EN 07:54



Active samples older than 7 days

- PCR 119 PCR B:H06
- PCR 119 PCR B:H04
- PCR 119 PCR B:H03
- PCR 119 PCR B:H02
- PCR 119 PCR B:H01
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- PCR119 O
- PCR 119 P
- PCR119 fo
- PCR119 Cl

- View
- View diagram
- New construct...
- Edit
- Delete

Google

Perspective: standard

Leads construct management

[Load Primer Order](#)
[Construct Management](#)

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Search by barcode

Search

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Basic concepts of PIMS

PIMS uses a few simple key concepts which can be linked together to model complex workflows

Targets

- Description of sequences, store annotations

Constructs

- Starting points for real experiments, link to targets

Samples

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

Experiments

- Take one (or more samples), produce new sample(s) as outputs





Experiments and protocols

A protocol is a reusable user-defined template describing what you record for your experiments.

Parameters

- Numerical values, free text values, T/F. *E.g.* incubation temperature or the number of PCR cycles; details of incubation conditions; was reagent added?

Input Samples

- Samples or reagents used when performing an experiment that you wish to track

Output Samples

- Samples or reagents produced when performing an experiment that you wish to track



Details of protocol: **OPPF TrialExpression**

Name

Remarks

Experiment type [Small scale expression](#)

Design new protocol based on this

Method

Inputs [Add new](#)

Parameters Add new: [Number](#) [Text](#) [Yes/No](#)

Output Samples [Add new](#)

Purified plasmid

Name

Amount

Category



Typing of PIMS items



Typing helps PIMS offer sensible choices: only a plasmid can be used for transfection experiments...

Samples

- Typed to show what they are

Input/Output samples for protocols

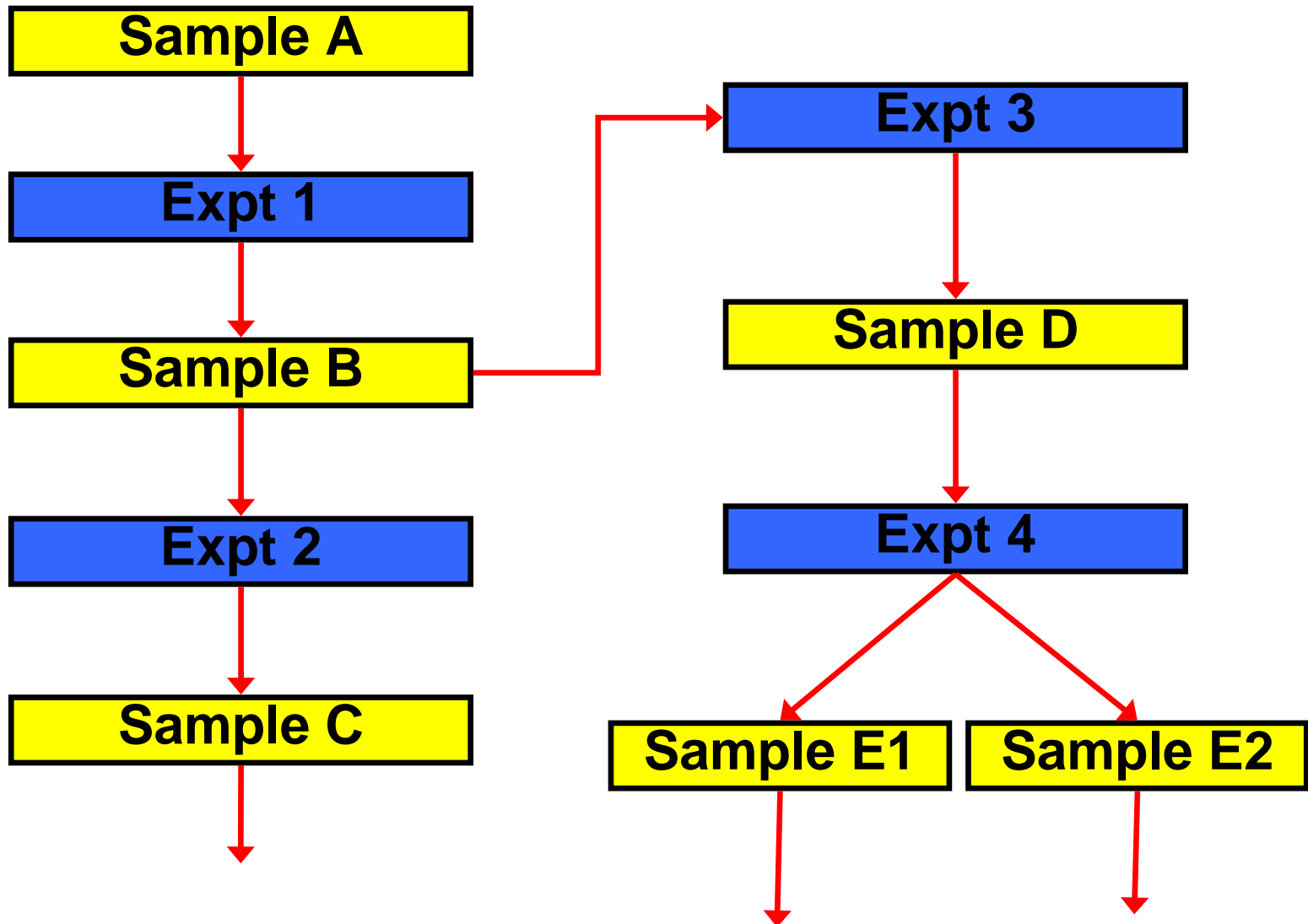
- State what type of sample can be used and what is produced

Experiments and protocols

- An experiment type is defined by its protocol. A protocol type links similar protocols together



Experiments & samples → Workflows





The PIMS holder (plate experiments)



A holder groups samples. This allows PIMS to perform plate experiments in groups

Samples

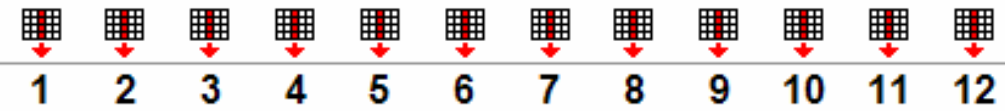
- For plate experiments output samples of previous experiment are mapped to input samples of next. (Provided sample type matches!)

User interface for plate experiments

- Gives graphical and spreadsheet views. Allows editing, reformatting and spreadsheet upload

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



A												
B												
C												
D												
E												

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

Can attach files to samples & experiments

Experiments can read/write data



OperonOrderFormPCR119Or29917
Microsoft Excel Worksheet
47 KB

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

Microsoft Excel - OperonOrderFormPCR119Or29917

File Edit View Insert Format Tools Data Window Help

A1 CUSTOMER CONTACT, SHIPPING + INVOICE DETAILS

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
8 City	Oxford	Oxford
9 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	AAGTTCTGTTTCAGGGCCCCGgaaacagaagagtggttttcaaggatataaccagg
3	OPPF4861F	AAGTTCTGTTTCAGGGCCCCGgaaacagcatgaaatccacccc
4	OPPF4864F	AAGTTCTGTTTCAGGGCCCCGgacagagttaccatggctggctg
5	OPPF4184F	AAGTTCTGTTTCAGGGCCCCGaagaagcaccacaagccccactg
6	OPPF4867F	AAGTTCTGTTTCAGGGCCCCGagcagccacctggaggactacagtg
7	OPPF4870F	AAGTTCTGTTTCAGGGCCCCGggcctggcttcacctttgg
8	OPPF4873F	AAGTTCTGTTTCAGGGCCCCGaccctgcggtgcctgagcc
9	OPPF4876F	AAGTTCTGTTTCAGGGCCCCGaaggaacatttacctggtaaatactttgg
10	OPPF4879F	AAGTTCTGTTTCAGGGCCCCGtctggagacagccataccatgtagc

Order details nr.5 / plate1 / plate2 / plate3

A cocktail of PIMS...

The image displays three overlapping screenshots of the PIMS web application interface, illustrating a 'cocktail' of different views and data.

Top-Left Screenshot: Shows the 'View Wells' page for 'OPTIC6289'. The browser title is '[PIMS] : [Xtal] : View Wells - Mozilla Firefox'. The URL is <http://www.opf.ox.ac.uk/biopims/Home.jsp>. The page features the 'bioPIMS' logo and navigation links like 'Home' and 'Logout'.

Top-Right Screenshot: Shows the 'Plate experiment: PCR119_1' page. The browser title is 'Plate experiment: PCR119_1 - Mozilla Firefox'. The URL is <http://localhost:8080/pims/View/ccp.api.Experiment.ExperimentGroup:20803>. The page includes the 'PIMS' logo and navigation tabs such as 'Basic details', 'Quick setup', 'Plate view', 'Spreadsheet view', and 'Files'.

Bottom Screenshot: Shows a detailed 'View Wells' page. The browser title is '[PIMS] : [Xtal] : View Wells - Mozilla Firefox'. The URL is <http://www.opf.ox.ac.uk/xtalpims/ViewWells.jsf?barcode=441300001935&name=441300001935-20030210-203201>. The page features a large image of a well with crystals, a 'Well Info' sidebar, and a grid of search results.

Well Info Sidebar:

Well Info

Plate: 441300001935

Well: A01-1

Date: Mon, 10 Feb 2003 20:32:01 GMT

Scores:

Date	Description	Name	Version
10/2/2003	Some Crystals	ALICE	

Annotate: [dropdown]

Taken by: Oasis 1700 (21°C)

Description: P1 + P2 Complex, Phi8, 5 mg/ml Block 5

Block: Block 5

Time course: [sequence of well icons]

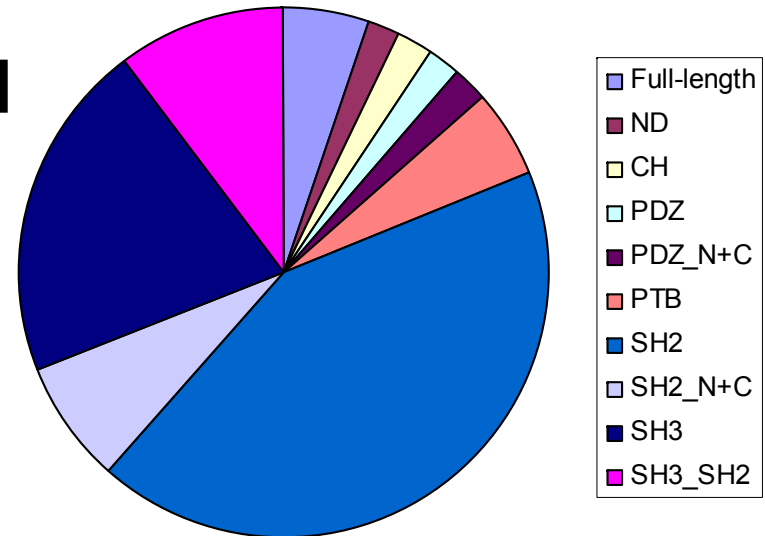




PCR107: OMC Plate 1

pOPINF (N-His)
96-well plate

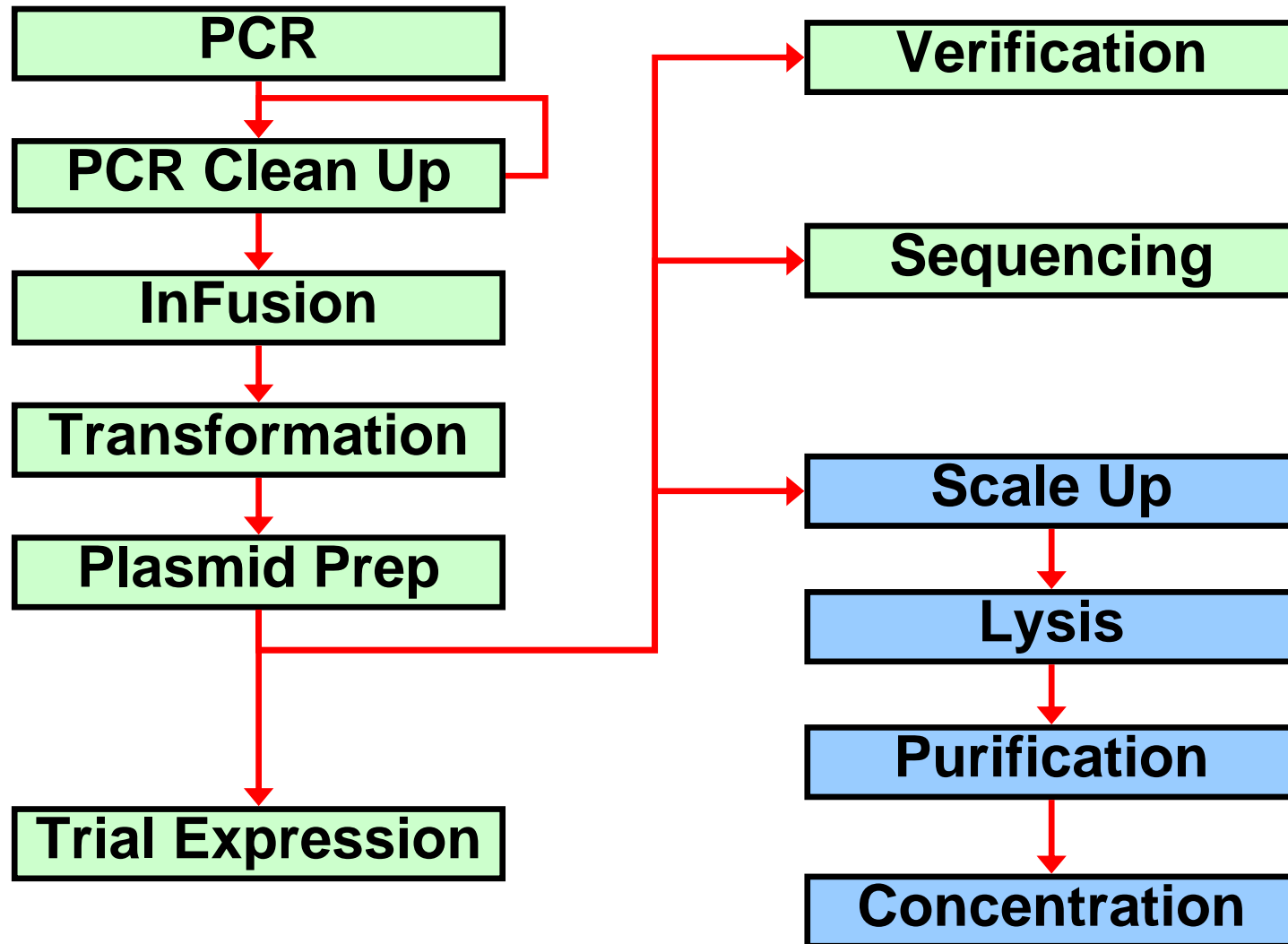
94% cloned
78% soluble expression
72% OVERALL SUCCESS



Now working on
PCR119: OMC Plate 2
Real dataset used for demo

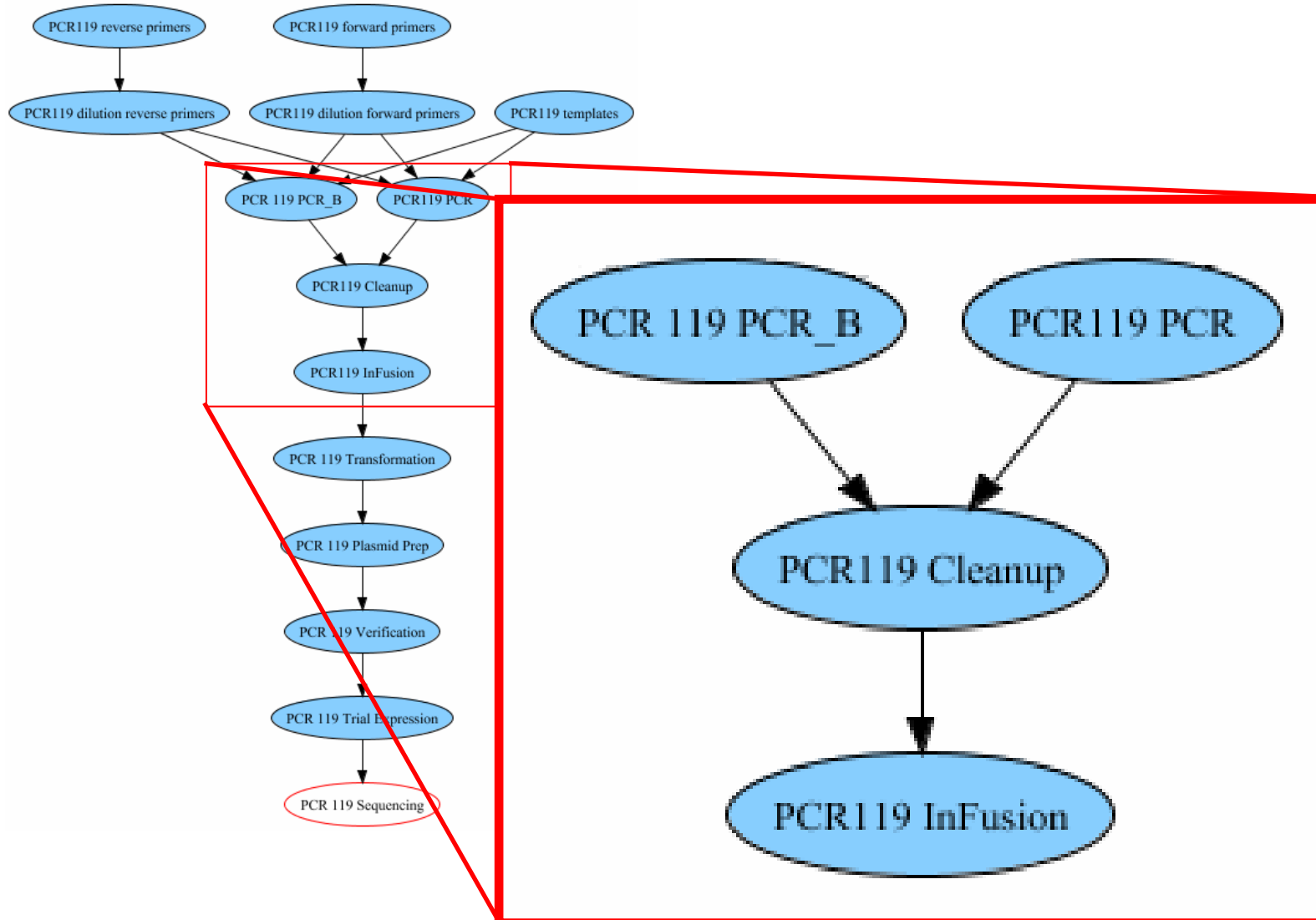


Protocols Used By PCR119





PCR119 workflow derived from PIMS





PIMS demonstration hardware



- Running on an average laptop
 - 1.7 GHz Pentium M Processor
 - 1GB memory
 - Windows XP SP2
- No external connection
 - Apache, Tomcat and Oracle all installed as services on this machine
 - Demonstrated using Mozilla Firefox
- Screen resolution limited to 1024x768
 - To suit projector



PIMS demonstration



- PIMS version 1.3
- Released last Friday (26/10/07)
- Running on Tomcat and Oracle
- Data for series of OPPF experiments (PCR119)

