

# Protein information Management System

Chris Morris  
STFC...

...and the PIMS development team



# Outline of talk

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- Who uses PiMS?
- Why use a LIMS?
- What PiMS does
- Forthcoming releases
- Sharing experimental data
- Future of PiMS
- Introduction to PiMS ....





# Who uses PiMS?

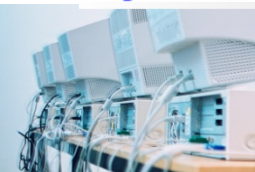
- MPSI 1064 Targets, 2536 Experiments, 3467 Samples,
- SSPF 392 Targets, 3709 Experiments, 1344 Samples
- OPPF using PiMS, no more data entry to Nautilus
- Adopted at IRB, Barcelona
- Free for academic use
- Commercial inquiry





# Why use a LIMS for protein production?

- Traceability, Searchability, Manageability, Continuity, Integration
- Flexibility, Future Proofing
- - lucky that we worked for **two** consortia
- Alternative 1: a combination of lab notebook and MS Office
- Alternative 2: Electronic Lab Notebook
- LIMS for: HTP, long term projects, scattered collaborations, automated work

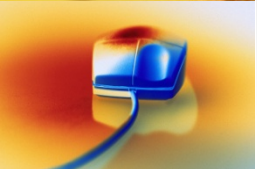




## PiMS 2.2 supports ....

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- work on ORF targets, complexes, promoters, protein from natural source ...
- Gateway, Infusion, ...
- individual experiments, groups of experiments, and work with plates
- Tracking samples
- Tracking reagents used





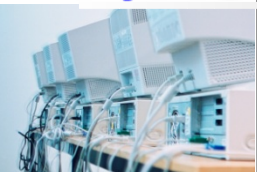
# Technologies used

- 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, ...





# Data Sharing



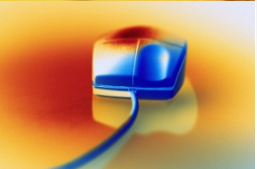
- “BBSRC expects research data generated as a result of BBSRC support to be made available ... BBSRC will provide support and funding to facilitate appropriate data sharing activities”
- “the absence in the PDB of detailed information regarding expression, purification and .. characterisation ... Such information on both successful and failed structural targets would be very useful...” PSI Assessment Panel, 2007.
- PiMS will enable publication and mining of experimental data



# Future work

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- Unified construct management
- Look and feel of a lab note book
- Scaling for large numbers of records
- More extensible

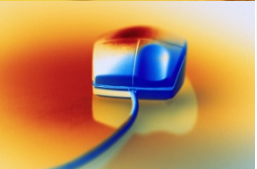




# The future of PiMS

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- Licenced like CCP4
- Grant applications to add new scientific functionality
- Will have central team at Harwell campus





# 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](#)

**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](#).

**Search by barcode**

Search

(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](#)

**Leeds construct management**

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

(Empty)

# Search by barcode

30405199304

Search



# Protein Information Management System 1.3

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Search by barcode

Search

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

Google

Perspective: standard

**Leads construct management**

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Construct Management

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**Search by barcode**

Search

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07:54



# Basic concepts of PIMS

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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

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

## Set Up Parameters

- *E.g.* incubation temperature or the number of PCR cycles; promoter sequence; was reagent added?

## Input Samples

- Samples or reagents used when performing an experiment that you wish to track, e.g. primers, host strains

## 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

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

## **Samples**

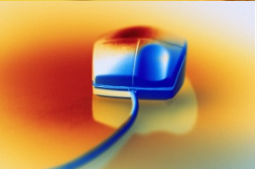
- Typed to show what they are

## **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





# The PIMS holder (plate experiments)

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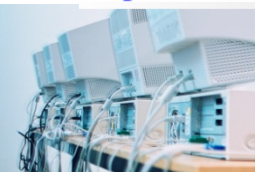
A holder groups samples. This allows PIMS to perform plate experiments in groups

## **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



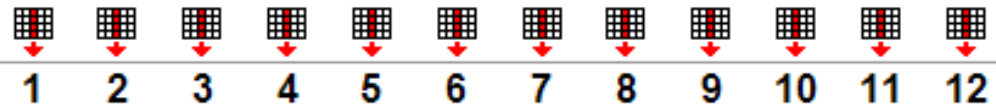
**Plate PCR119 Cleanup, well A1**  
**Target OPPF3926**

Kit: 90.0uL, **Unspecified**

PCR product: 50.0uL PCR119 PCR:A01

Checked on gel?: Yes

Status: To be run

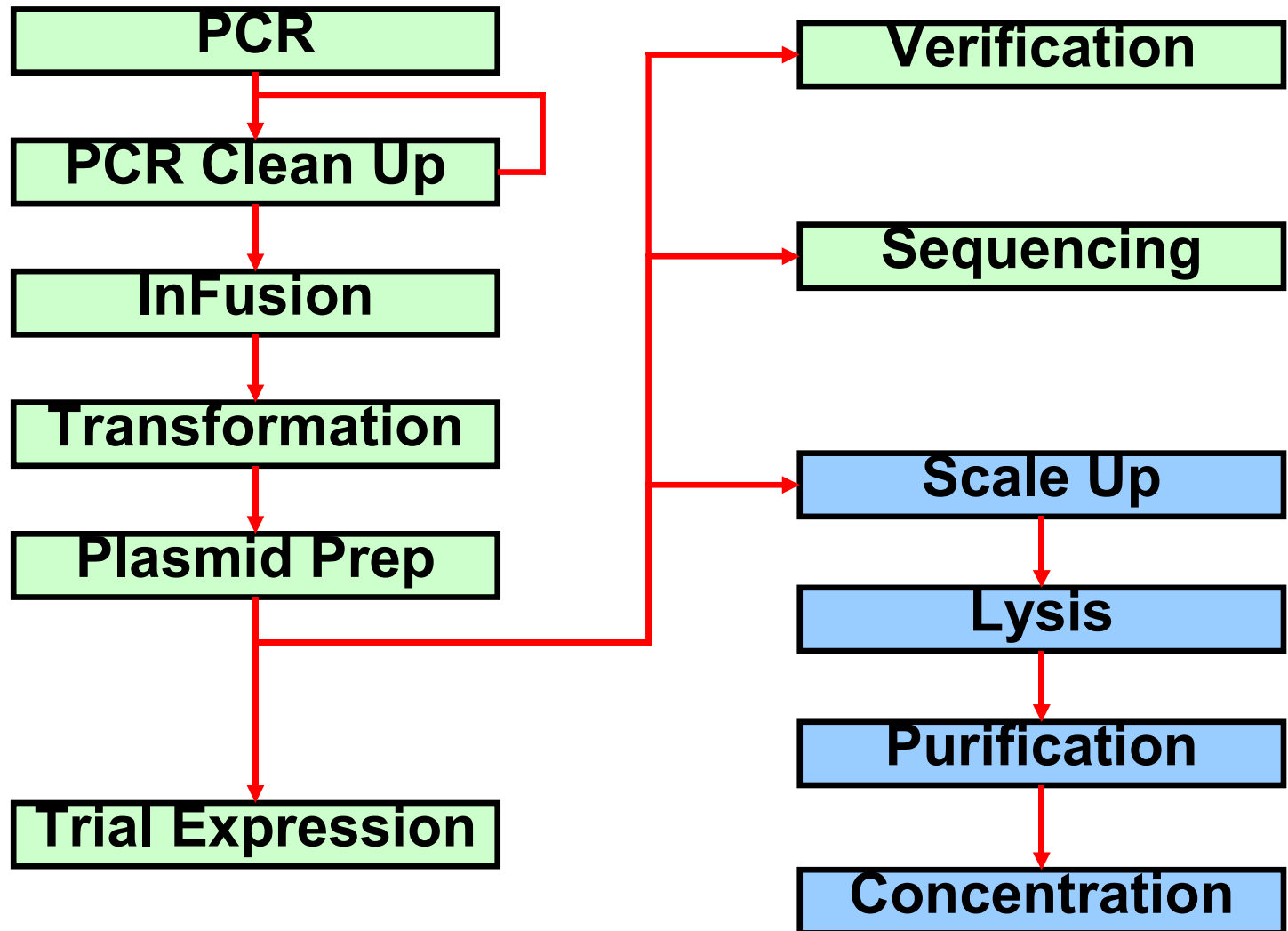


**Basic details** | **Quick setup** | **Plate view** | **Spreadsheet view** | **Files**

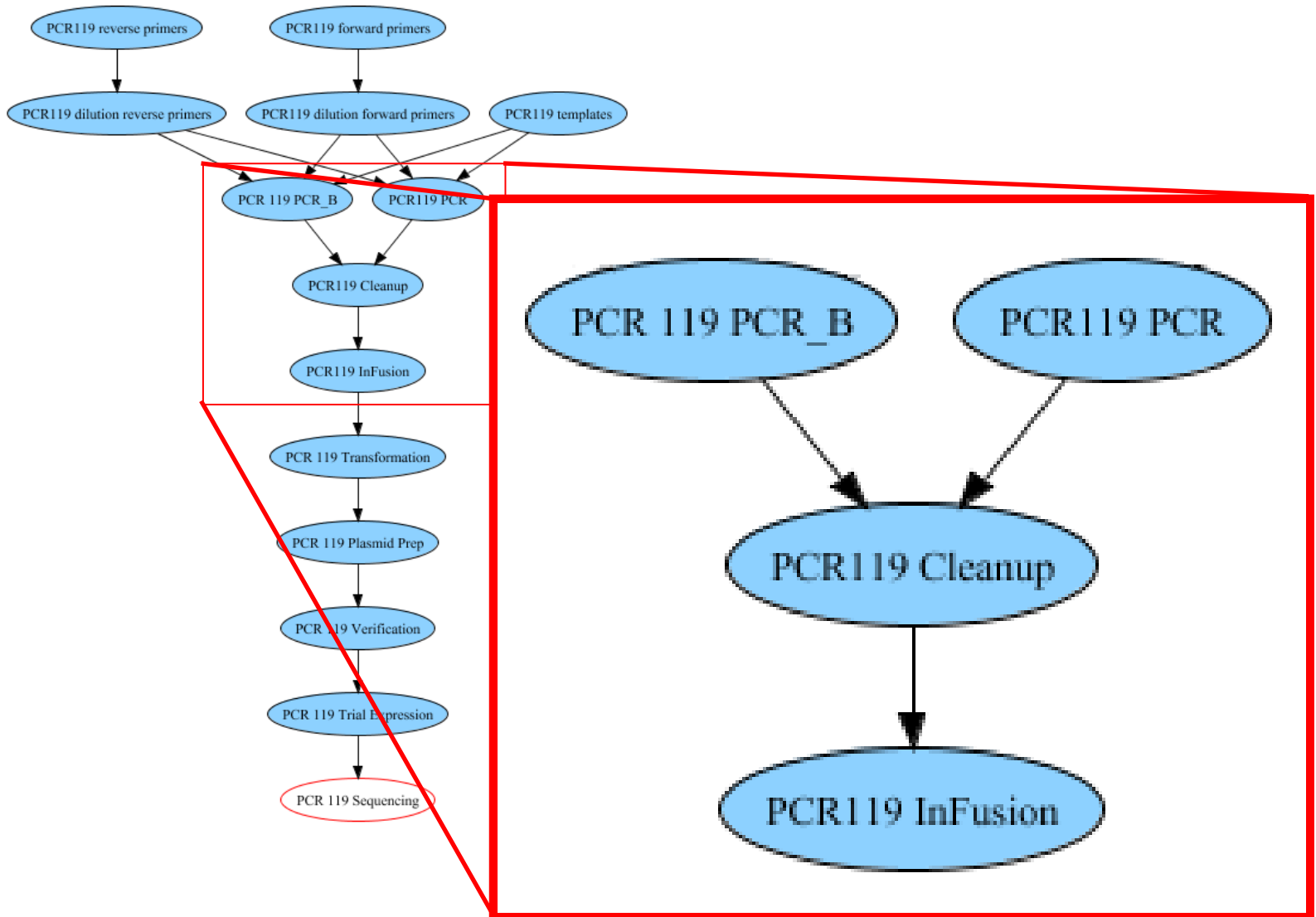
Tray	Row	Col	Target	Status	Output	Kit	
						Sample	Vol uL
PCR119 Cleanup	A	1	OPPF3926	To be run <input type="button" value="v"/>	<a href="#">PCR119 Cleanup:A01</a>	(None)	90.0
PCR119 Cleanup	B	1	OPPF4861	To be run <input type="button" value="v"/>	<a href="#">PCR119 Cleanup:B01</a>	(None)	90.0
PCR119 Cleanup	C	1	OPPF4864	To be run <input type="button" value="v"/>	<a href="#">PCR119 Cleanup:C01</a>	(None)	90.0
PCR119 Cleanup	D	1	OPPF4184	To be run <input type="button" value="v"/>	<a href="#">PCR119 Cleanup:D01</a>	(None)	90.0
PCR119 Cleanup	E	1	OPPF4867	To be run <input type="button" value="v"/>	<a href="#">PCR119 Cleanup:E01</a>	(None)	90.0
PCR119 Cleanup	F	1	OPPF4870	To be run <input type="button" value="v"/>	<a href="#">PCR119 Cleanup:F01</a>	(None)	90.0
PCR119 Cleanup	G	1	OPPF4873	To be run <input type="button" value="v"/>	<a href="#">PCR119 Cleanup:G01</a>	(None)	90.0

**Can attach files to samples & experiments**

# Basic protocols used at OPPF



# A workflow derived from PIMS



# Acknowledgements

- Johan van Niekerk, Dundee
- Susy Griffiths, YSBL
- Anne Pajon, EBI
- Ekatarina Pilicheva, Marc Savitsky, Jon Diprose, Robert Esnouf OPPF
- Bill Lin, Ed Daniel, Peter Troshin STFC
- ... all who told us what PiMS should do