



Why PiMS?

Chris Morris

STFC Daresbury Laboratory...

...and the PIMS development team

PiMS Outline of talk



- **Why use a LIMS?**
- **Use of PiMS for real projects**
- **PiMS concepts**
- **xtalPiMS for crystallization**
- **Future work**



- Traceability, Searchability, Manageability, Continuity, Integration
- Flexibility, Future Proofing
- - lucky that we worked for **two** consortia
- LIMS especially for: HTP, long term projects, scattered collaborations, automated work, services



- Free format: MS Office, ConturELN, wiki
- Structured: general purpose LIMS
 - or Customer Relationship Management system
- Molecular Biology aware: Vector NTI, PDB, PiMS



- Closure of many in-house R&D groups
- Sharing risk with academic groups
- Market in drug candidates
- Product could includes methods
- Use of Contract Research Organisations

Need for collaborative knowledge management solutions

PiMS Potential problems with LIMS



■ 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”





	Setup	Entry	Retrieval	Loss
Paper	+	+	+++++	+++++
MS Office	++	++	++++	++++
ELN, Wiki	+++	+++	+++	+++
LIMS, CRM	++++	++++	++	++
PiMS	++	+++	+	+

PiMS Who uses PiMS?



- MPSI 1064 Targets, 2536 Experiments, 3467 Samples
- SSPF 392 Targets, 3709 Experiments, 1344 Samples
- OPPF 352 Targets, 20,559 Experiments, 18,714 Samples
- 2012 PiMS adopted at CalTech, Minsk, Prague, ...
- XtalPiMS adopted in OPPF, Oulu.
- **PiMS Free for small academic groups (up to 6)**
- **For PiMSPro, contact Emerald BioSystems**

What do they say about PiMS?



17 replies / 18 academic licenses

- 4: "I love PiMS" / "PiMS is brilliant" / "of great use for us" / "it is a key application that we do not want to miss anymore!"
- 4: "time investment needed to start using it" / "too much time had to be put in initially" / "energy needed to get into it" / "the learning curve was too steep for us"

PiMS Technologies used in PiMS



- **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**

- 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,



- work on ORF targets, complexes, promoters, protein from natural source ...
- Gateway, Infusion, ...
- Site Directed Mutagenesis
- individual experiments, groups of experiments, and work with plates
- Tracking samples: freezer view
- Booking instruments
- Crystallogenes in xtalPiMS extension

PiMS Access rights



- **Data can be:**
- **Private (MS Word)**
- **Public (MediaWiki)**
- **Managed access...**
- **Each PiMS record belongs to a “lab note book”**
- **Each user can write in one or more lab note books**
- **Your lab note book may be:**
- **Private to you**
- **Or readable by your supervisor**
- **Or shared with colleagues**

PiMS PiMS uses simple key concepts



■ Complexes & Targets

- Descriptions of proteins and complexes
- Can contain bioinformatics annotations

■ Constructs

- Starting point for real experiments
- Describes actual sequences

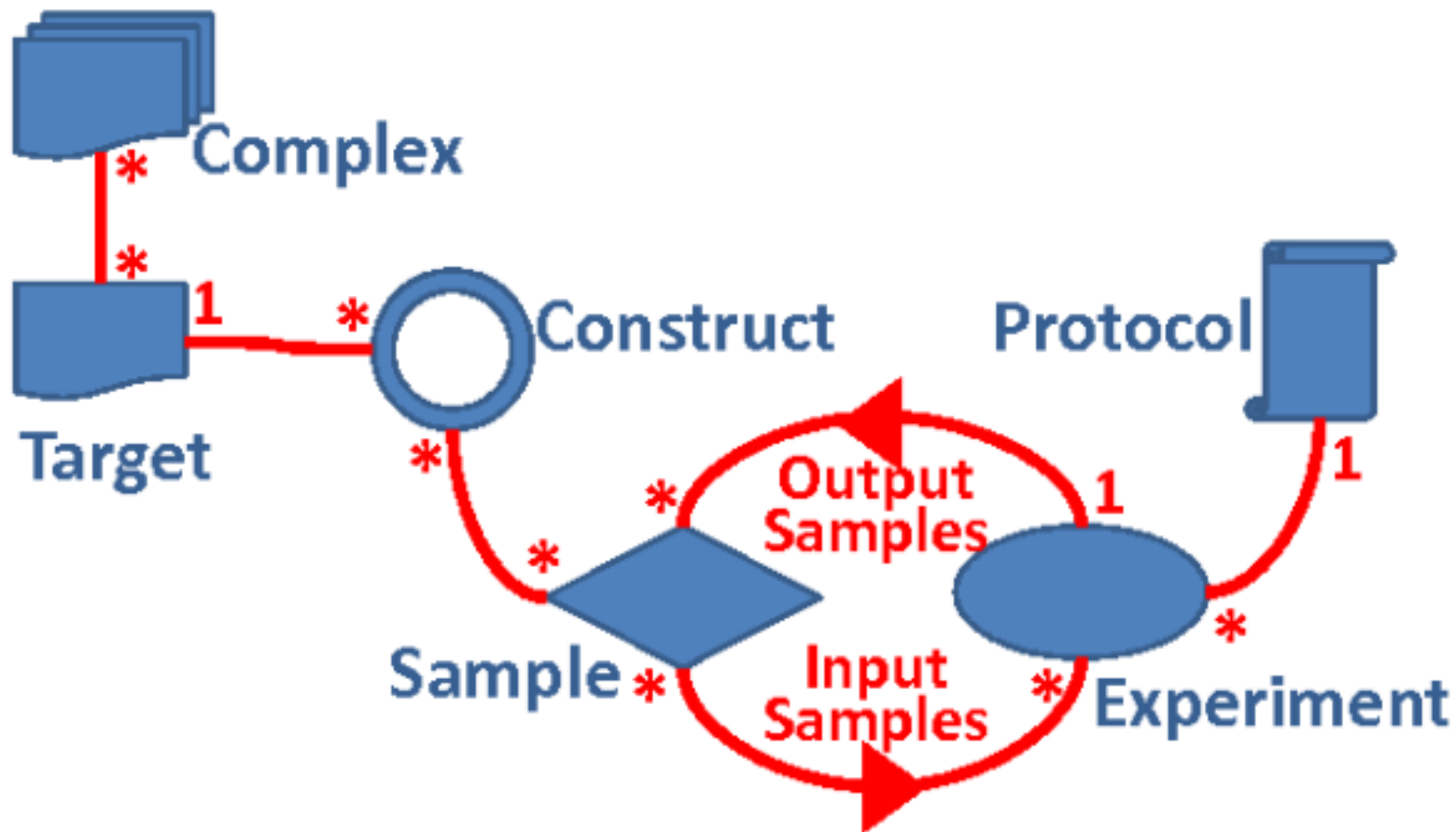
■ (Typed) Samples

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

■ Experiments & Protocols

- Consume (input) and produce (output) samples

PiMS How it all links together





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[Log out c Morris](#)
[Target](#)
[Experiment](#)
[Sample](#)
[User](#)
[Help](#)
[History](#)

[Search](#)
 Perspective: standard

Targets :
T000004

[New experiment](#)
[New construct](#)
[Diagram](#)
[Delete](#)
[New Synthetic gene](#)

<<
 <
 Dec 2012
 >
 >>

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	31					

Basic Details

Sequences
 Protein sequence and Translated DNA sequence do not match

[Alignment](#) between translated DNA sequence to recorded protein sequence

[DNA sequence](#)

ATGACACACGTTTCCAGAG AAAATTTCTTTTCAACACAG GCGCGGCGGCGGCGGCTTCT ATTTGGTACATGGCTGTAC TTCCATGGTTCTCANTCAG
 CTACCACAGGAGACACAGCG OCTTCAGCAGCACCAGCGC TAATGTCTCAGCGCTAACG CACCCAGGTAGAAAGACT AAAGCCAGTTAGGATTAT
 Length: 1323 %GC: 42.78 [Fasta Pop-up](#) Reverse complement [Pop-up](#)

[Protein sequence](#)

MTHVSRKFLPTTGAAGAS ILVHOCTSNQSQSATTGEA PSAAPAAVSAANAFVETT KALGFIPITDAAPLIIARE KOFFAKYQMTDIEVIKQESH
 PYTRDLKIGSSGGGIDGAH ILSPMPYLMTINDKVPNYIL ARNTNGQAIQVAEKFEELN VNLESKSLKDAIKAKADEK ALKMGITPPGGTHDLNRYM
 Length: 440 Weight (Da): 48,475.6 Extinction: 77515.0 Abs 0.1%: 1.599 pI: 8.34
[Fasta Pop-up](#)

[Make changes...](#)

Constructs
 Design new Construct

Experiments
 New Experiment

Items found, displaying all items. 1

Date	Status	Experiment	Protocol	Milestone
12 December 2012 05:50:00 GMT	To_be_run	Small scale expression-Sse c Morris 1:G01	PIMS Trial Expression	
11 December 2012 17:45:01 GMT	To_be_run	T000004.full-PCR	PIMS PCR	
11 December 2012 17:47:52 GMT	To_be_run	T000004.full-Ligation c Morris 1	PIMS Ligation	

Construct: starting point for experiments, links to target



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Targets : T000004 :

Construct: T000004.full

[Diagram](#)
[Delete](#)
[Milestones](#)
[New SDM](#)
[Primers](#)

Basic Details

Page Number	PN3-12	Scientist	none
Construct Name	T000004.full	Comments	
Description	full lenght	Owner: MolBio-Core	

Make changes...

Forward Primer: T000004F1

Reverse Primer: T000004R440

Full sequence

GCAATTCGGATCCTCACTAG ACTTTTTGATTTTCAAACT ATTAAAGTATTCCTC

Length: 55 Tm °C: 70.2 %GC: 30.9 Molecular Mass: 16,842 [Fasta pop-up](#)

Overlap region

GACTTTTTGATTTTCAAAC TATTTAAGTATTCCTC

Length: 36 Tm °C: 60.4 %GC: 22.2

5'-Extension

GCAATTCGGATCCTCACTA

Make changes...

Insert

Proteins

Experiments [New Experiment](#)

Images

Attachments

Sample: has type, owner, location



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Samples :

T000004.full-Plasmid

[Barcode](#)
[Move](#)
[Diagram](#)
[Sample History Report](#)
[Delete](#)
 Can't divide sample - set an amount first.
 [Help](#)

Basic Details

Page Number		Stock available	@ Yes
Name*	T000004.full-Plasmid		No
Amount	0.0uL	Use by date	13 December 2012 14:17:52 GMT
Row		Assigned to	
Column		Lab Notebook	MolBio-Core
Sub Position		Details	

Make changes...

Sample categories [Search/Add](#)

Recipe and/or components

Was Output from Experiment: [T000004.full-Ligation cmorris 1](#)

Parameter	Value
Buffer type*	
Enzyme*	Quick Ligase
Incubation conditions*	
Total Volume (uL)*	21

Make changes...


Used as Inputs to Experiments ...


Dec 2012						
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	31					



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[Search](#)
 Perspective: standard


Protocols :



PIMS Bicistronic InFusion

[Diagram](#)
[New single experiment](#)
[New experiment group](#)
[New plate experiment](#)

[Export](#)
[Copy](#)
[Can't delete](#)
[Help](#)

Basic Details

Page Number		Objective	Capture PCR Product into pOPIN vectors
Name*	PIMS Bicistronic InFusion	Lab Notebook	
Experiment type	Cloning	Is for use	Yes
Instrument type			
Remarks	Default set of protocols for PIMS;		
Details	Capture PCR Product into vectors		

Method

Inputs

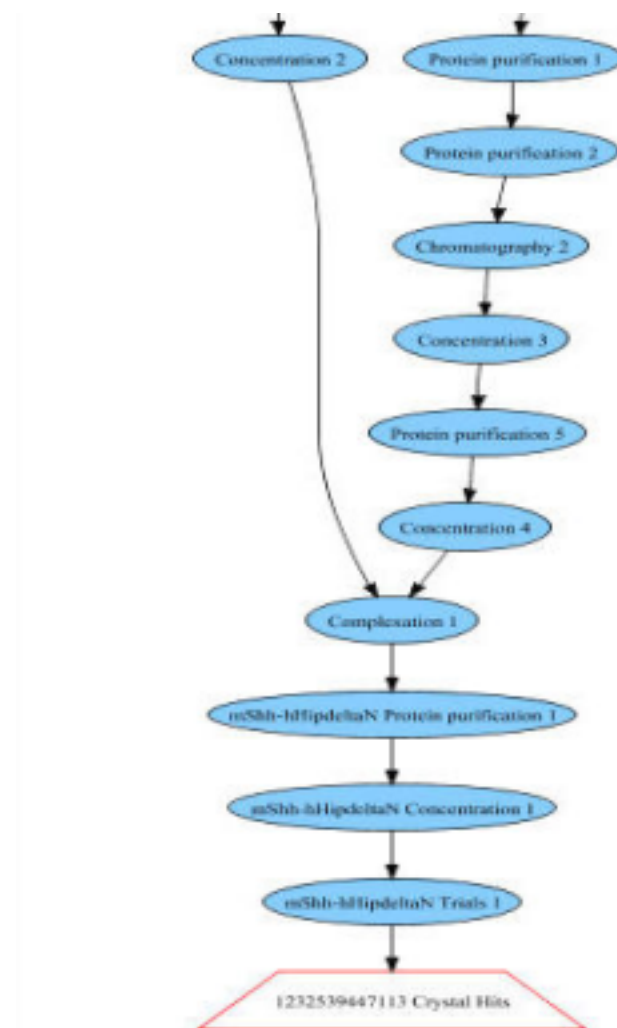
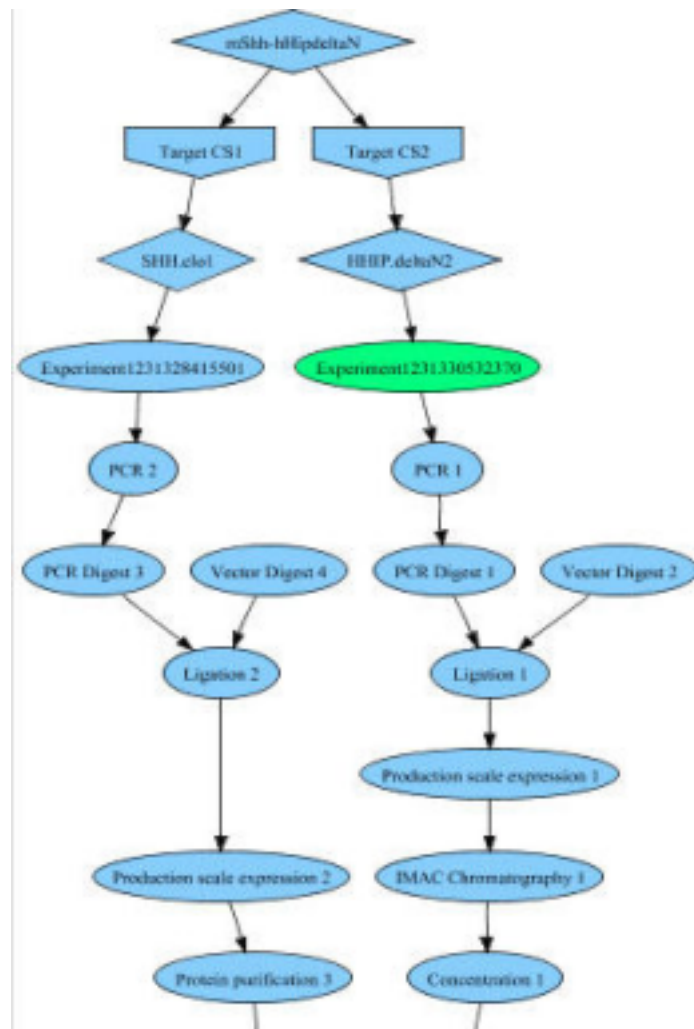
Name	Default amount	Category
PCR Product A	2.0uL	Nucleic acid
PCR Product B	2.0uL	Nucleic acid
Vector	1.0uL	Vector

Group level parameters

Set-up parameters

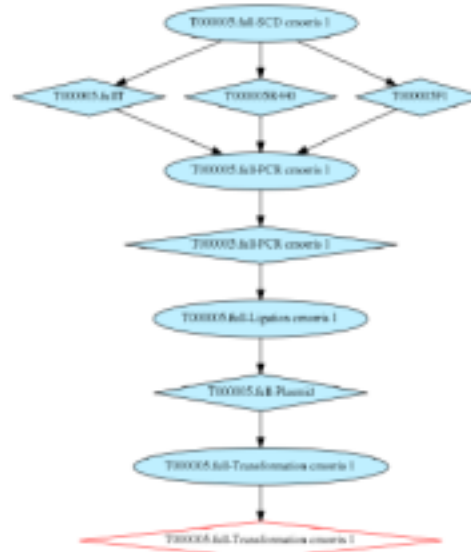
Result parameters

Output Samples



Simple reports of how samples are made

PiMS Sample History Report Thu Dec 13 14:45:43 UTC 2012



Experiment : T000005.full-SCD cmorris 1-SPOT Construct Primer Design

Protocol	SPOT Construct Primer Design
Scientist	cmorris
Start date	13/12/2012
End date	13/12/2012
Parameters	Forward Tag: GIEGR Reverse Tag:

Experiment : T000005.full-PCR cmorris 1-PiMS PCR

Protocol	PiMS PCR
Scientist	cmorris
Start date	13/12/2012
End date	13/12/2012
Inputs	Forward Primer: T000005F1 Reverse Primer: T000005R440



The xtalPiMS home page

[xtalPiMS] : Home - Mozilla Firefox

File Edit View History Bookmarks Tools Help

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

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xtalPiMS

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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	06/01/2010 19:20	Salt Crystals	dan	-	human	-
441300303567	E10.1	06/01/2010 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	Organisation
Adenovirus IVa2	erika	
Aeropath	ray	
AVV	dave	
AMPA	radu	

Done

Boxes show latest updates for projects that you have access to

[xtalPIMS] : View Trial Drops - Mozilla Firefox

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tal | http://www.oppl.ac.uk/xtalpims/ViewTrialDrops.jsp?barcode=441300356020&name=441300356020-20060614-19

Google

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Navigation - plate 441300356020

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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

16/5/2009 walter Crystals

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](#)

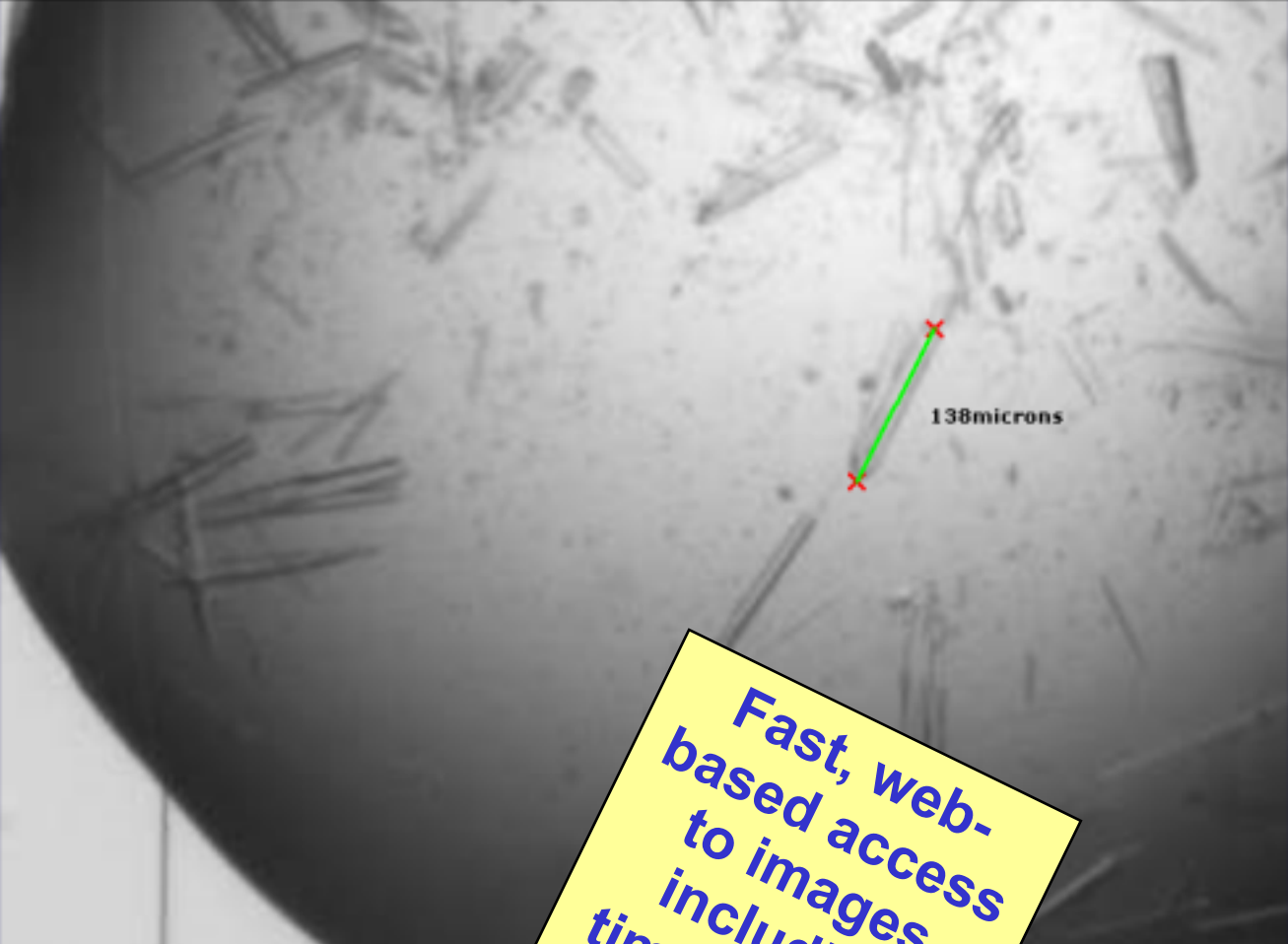
Earliest Latest



[Full time course...](#)

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

PIX Zoom: 200% Annotate:



Fast, web-based access to images including time courses

Done

[xtaPIMS] : View Trial Drops - Mozilla Firefox

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tal | http://www.oppl.ac.uk/xtalpims/ViewTrialDrops.jsp?barcode=441300356020&name=441300356020-20060814-19

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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
DbClick	Zoom in on clicked pixel
Ctrl+DbClick	Zoom out on clicked pixel

includes time courses



- Better support for the lab manager
- Reports
- User management
- Better usability, to improve compliance
- Investment by Emerald BioSystems
- Academic funding:
 - “BioMedBridges” EU grant for data integration
 - Oulu University contributing crystal treatment
 - CCP4 funding to support academic users



- Mobile clients
- DNA chemistry
- Reagent stocks
- Bioinf for construct design

“Outlook for structural biology”



A unified and extensible set of software tools for molecular biology, offering seamless data transfer and a consistent user experience, from target selection to extraction of biological significance from the structure

? -> PiMS -> xtalPiMS

-> ISPyB -> Xia2 -> CCP4 ->

?

PiMS Acknowledgments



■ 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 people

■ Ian Berry

■ PiMS and xtalPiMS users

■ Emerald BioSystems



Graphical interface for plate experiments

Plate PCR119 Cleanup, well A1

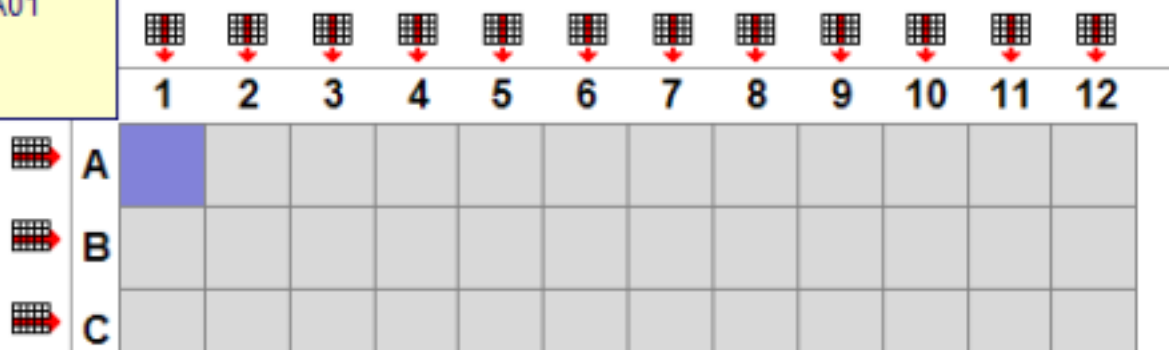
Target OPPF3926

Kit: 90.0uL, **Unspecified**

PCR product: 50.0uL PCR119 PCR:A01

Checked on gel?: Yes

Status: To be run



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

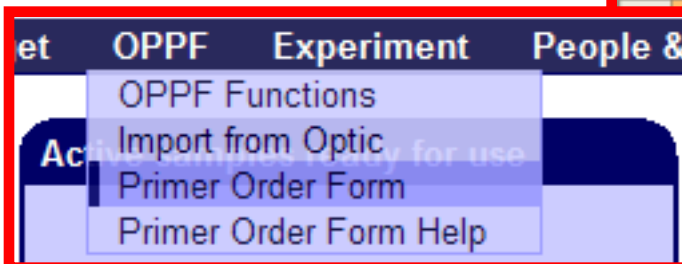
Tray	Row	Col	Target	Status	Output	Kit	
						Sample	Vol uL
PCR119 Cleanup	A	1	OPPF3926	To be run ▼	PCR119 Cleanup:A01	(None)	90.0
PCR119 Cleanup	B	1	OPPF4861	To be run ▼	PCR119 Cleanup:B01	(None)	90.0
PCR119 Cleanup	C	1	OPPF4864	To be run ▼	PCR119 Cleanup:C01	(None)	90.0
PCR119 Cleanup	D	1	OPPF4184	To 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

Experiments can read/write data



OperonOrderFormPCR119Or29917
Microsoft Excel Worksheet
47 KB



CUSTOMER CONTACT, SHIPPING + INVOICE DETAILS		
A	B	C
Details	Ship to	Bill To
Name	Ray Owens	Finance Department
University/Company	Wellcome Trust Centre for Human Genetics	Wellcome Trust Centre for Human Genetics
Department	OPPF	Accounts Division
Street	Roosevelt Drive	Roosevelt Drive
City	Oxford	Oxford
Post code	OX3 7BN	OX3 7BN
	UK	UK
Phone No.	01865 287500	01865 287500
Email	ray@strubi.ox.ac.uk	ray@strubi.ox.ac.uk
SEQUENCE		
1 OLIGO ID	SEQUENCE	
2 OPPF3926F	AAGTTCTGTTTCAGGGCCCCGgaaacagaagagtggttttcaaggatataaccagg	
3 OPPF4861F	AAGTTCTGTTTCAGGGCCCCGgaaacagcatgaaatccacccc	
4 OPPF4864F	AAGTTCTGTTTCAGGGCCCCGccagagtttaccatggctggctg	
5 OPPF4184F	AAGTTCTGTTTCAGGGCCCCGaagaagcaccacaagccccactg	
6 OPPF4867F	AAGTTCTGTTTCAGGGCCCCGagcagccacctggaggactacagtg	
7 OPPF4870F	AAGTTCTGTTTCAGGGCCCCGggccgtggcttcaccttttgg	
8 OPPF4873F	AAGTTCTGTTTCAGGGCCCCGaccctgcggtgccttgagcc	
9 OPPF4876F	AAGTTCTGTTTCAGGGCCCCGaaggaaacatttaccctggtaaatcatttacccttttgg	
10 OPPF4879F	AAGTTCTGTTTCAGGGCCCCGctggagacagccataccatgtagc	

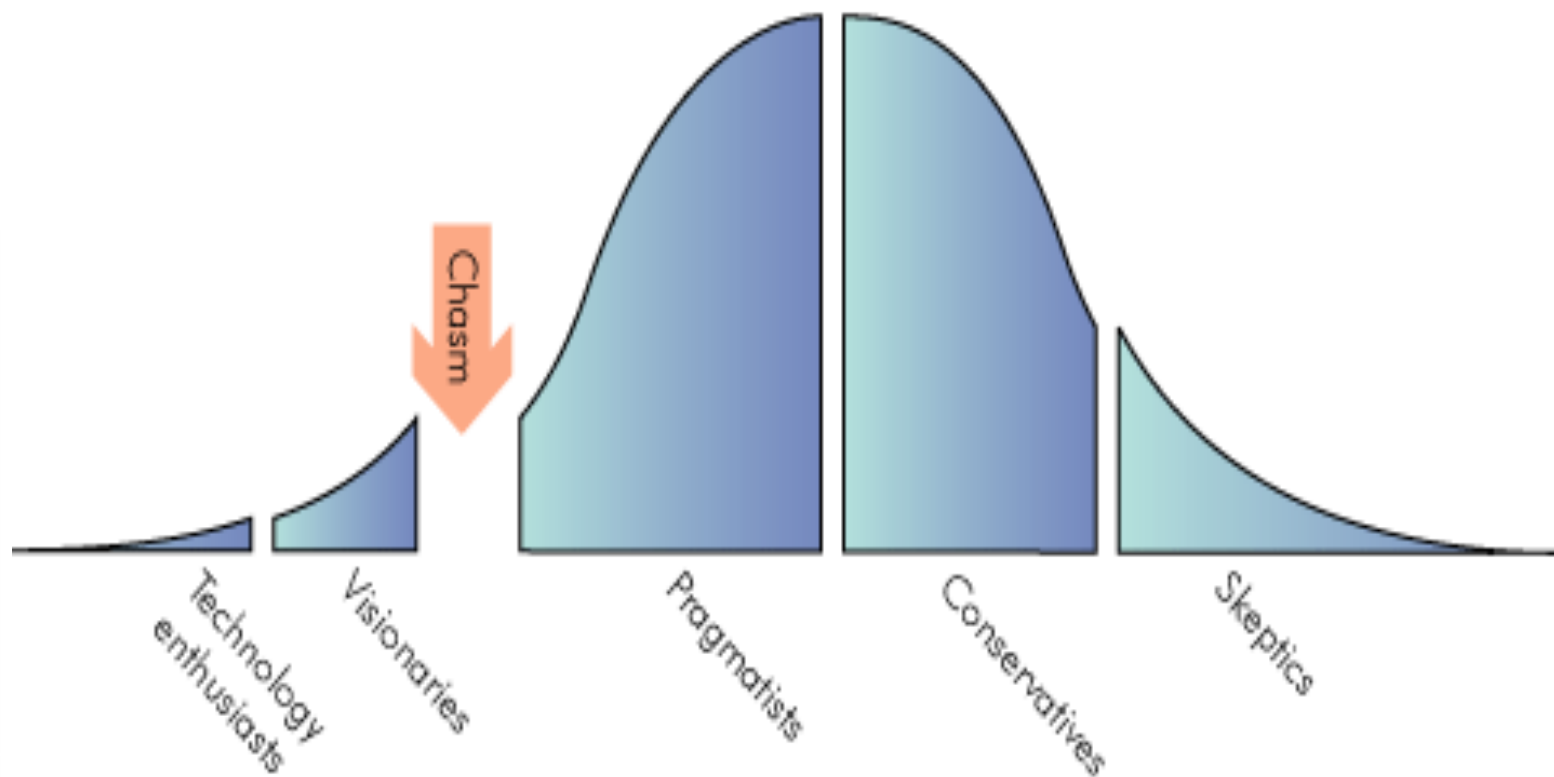
Export options: CSV | Excel



	Free form	Structured	Mol.Biol. aware
Private	MS Word	MS Excel	VectorNTI
Controlled	ConturELN	Nautilus SugarCRM	PiMS
Public	MediaWiki	-	PDB



- 17 replies / 18 academic licenses
- 5: *never able to get a good **installation***
- 5: *one useful **addition** would be ... / very small incremental improvements / increase the bioinformatics tools / plugins / A friendly browser-based user management would be very helpful*
- 4: *I **love** PiMS / PiMS is brilliant / of great use for us / it is a key application that we do not want to miss anymore!*
- 4: *time investment needed to start using it / too much time had to be put in initially / energy needed to get into it / the **learning curve** was too steep for us*
- 2: *finding the right way to use it / We think that some **training** would be needed now.*
- 2: *weird java error messages / there are still many (small) **bugs***
- *until we are **told** to use it*

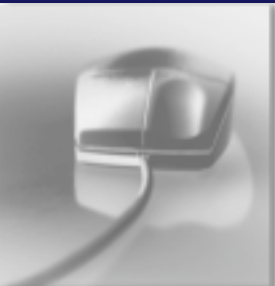


- The greatest credibility gap is from visionaries (~5%) to pragmatists (~33%)
- This is the stage that PiMS is at.

Contradictions in requirements = key design challenges



- 1) Easy installation v. reliable backup
- 2) 139 feature requests v. “day to day problems of finding the right way to use it”
- 3) Scientists' autonomy v. sharing laboratory space

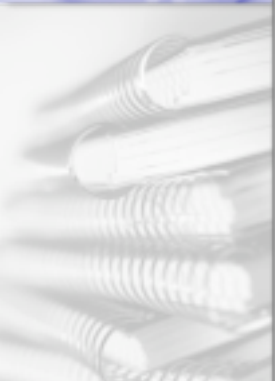


I won't tell them to use it

v.



Please write down start/finish times so others may use the shaker when it is free





If you record

- (earlier) I want to use the Akta tomorrow
- I used some of the standard elution buffer
- I used up aliquot T00057.full-supernatant
- I stored aliquot T00057.full-Ni

Then you have actually made a full record of the science done.



- Highlight “next step”
 - Module: Booking instruments
 - Module: Freezer index
 - Module: Reagent stocks
 - Module: Archive of files
 - Module: Protocols
 - “Please fix” page
- “Outlook for structural biology”