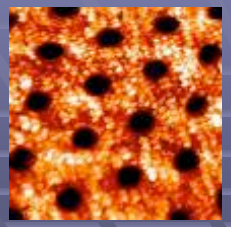
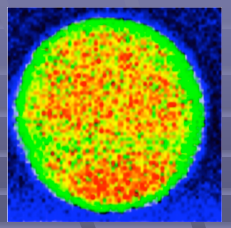
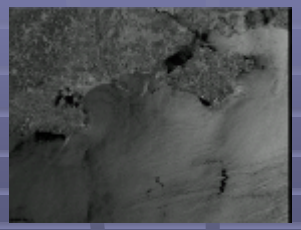
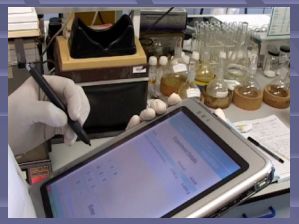
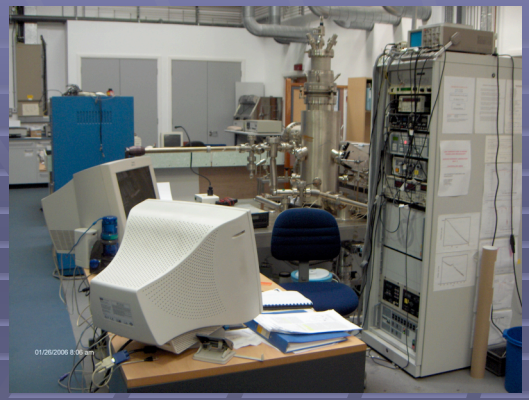




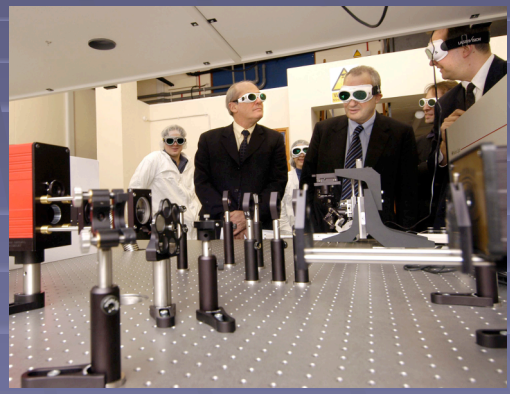
Smart Lab 2.5



The digital future of laboratory Chemistry

Jeremy G.Frey
School of Chemistry
University of Southampton, UK





Talk

- Laboratory Research
- Laboratory Notebooks
- Blogs and Blogjects
- Publication@Source

Jeremy G. Frey
University of Southampton

Research Space
UCB Guidelines

- Research space is a more complex problem. Changes over the past decade have no doubt been even more profound for research space than office space: but those changes are unique to each discipline, and to identify and characterize them would be a significant project in itself…..

UCB Space Study

Space for model building…..

Jeremy G. Frey
University of Southampton

The tea room is the ‘heart’ of the department - plans to create a more interdisciplinary equivalent for the Life Science Interface ut still only serves a local function

Growing need for the global (virtual) equivalent of the “Tea Room”

Social Space? Space for Discussions?

Jeremy G. Frey
University of Southampton

The CombeChem Project

- End to End linking of data and information
  - Publication@Source
- So collect data with regard to how it could eventually be used
  - Make sure the metadata is of high quality
  - Record properly at source in Digital Form
- The Chemistry Lab
  - People & Machines working together

Jeremy G. Frey
University of Southampton

Combechem

Smart Lab

E-Malaria

R4L

Instruments on the Grid

e-Bank

Statistics

BioSimGrid

Jeremy G. Frey
University of Southampton

If only I knew exactly how she did this experiments

I wish I had recorded things at the start the way I do now…..

I know all this supplementary information could be useful but will people really remember the format? Is it worth all the hassle?

I wish I could get the numbers from this graph - the pdf is not much use.

Typical Laboratory

Jeremy G. Frey
University of Southampton

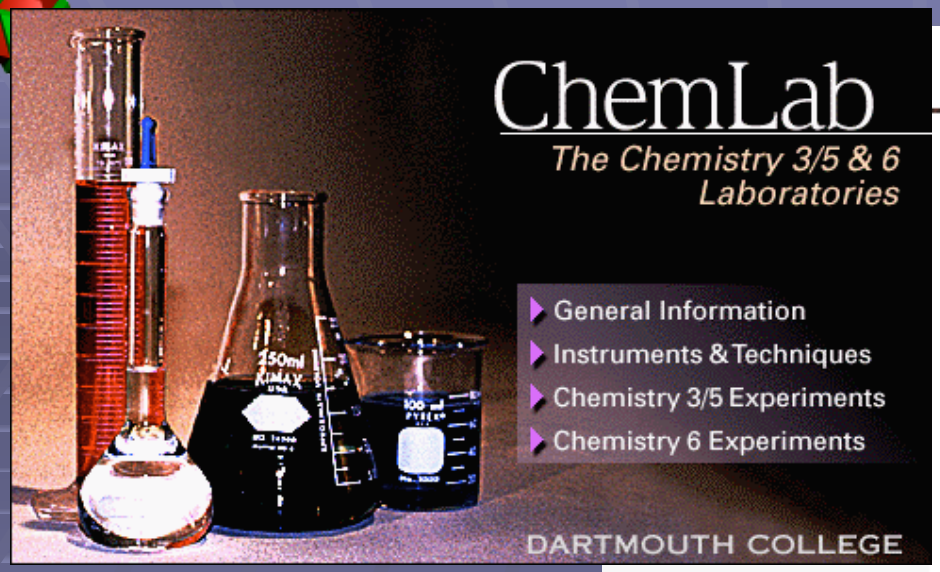
I am sure we collected that information a few years ago…

The details should be in her thesis……

Can you read what he says here….?

Can you find the file of data that were used to make the plot?

Some of these problems are due to the lack of information recorded at the time. Others are due to loss of information over time.



Permanent, documented and primary record of laboratory ***observations***

How to Keep a Notebook

One of the most useful skills you will acquire in the laboratory is the proper use of a laboratory notebook. Notebooks, or other formally kept records, are an essential tool in many careers, ranging from that of the research scientist to that of the practicing physician. The effort invested in developing good habits of notebook use will be amply repaid for students who pursue a future in the basic or applied sciences. Experience has indicated that skillful notebook use is developed by most students only through continued special effort--it does not come naturally. Some of the main principles of sound notebook use are outlined below.

The laboratory notebook is a permanent, documented, and primary record of laboratory observations. Therefore, your notebook will be a bound journal with pages that should be numbered in advance and never torn out. A notebook will be supplied to you before the first laboratory period. Write your name, the name of your TA, and your lab section on the cover of your notebook. All notebook entries must be in ink and clearly dated. No entry is ever erased or obliterated by pen or "white out". Changes are made by drawing a single line through an entry in such a way that it can still be read and placing the new entry nearby. If it is a primary datum that is changed, a brief explanation of the change should be entered (e.g. "balance drifted" or "reading error"). No explanation is necessary if a calculation or discussion is changed; the section to be deleted is simply removed by drawing a neat "x" through it.

Safety
General Rules
Safety Equipment
Safety Hazards
[illegible] Procedures

Resources
Applets
General FAQ
Uncertainty

ChemLab Home

29 Jan 2007

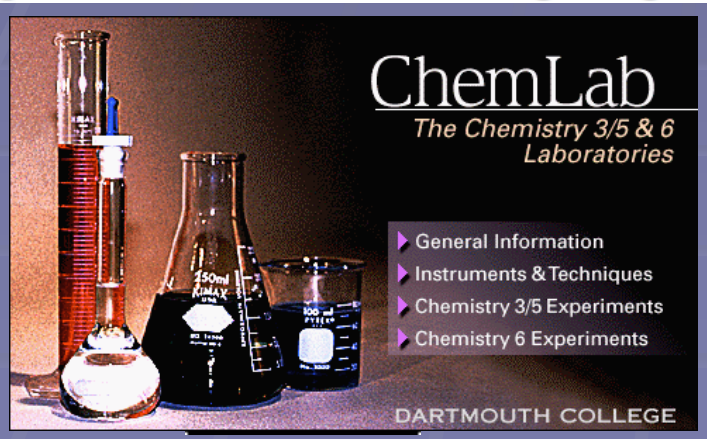
necessary if a calculation or discussion is changed; the section to be deleted is simply removed by drawing a neat "x" through it.

In view of the fact that a notebook is a primary record, data are not copied into it from other sources (such as this manual or a lab partner's notebook, in a joint experiment) without clear acknowledgment of the source. Observations are never collected on note pads, filter paper, or other temporary paper for later transfer into a notebook. If you are caught using the "scrap of paper" technique, your improperly recorded data may be confiscated by your TA or instructor at any time. It is important to develop a standard approach to using a notebook routinely as the primary receptacle of observations.

Each week at the beginning of lab lecture, you will t… your prelab problems from the manual for grading. P… problems not turned in at the beginning of lab lecture will be

Observations are never collected on note pads, filter paper or other temporary paper for later transfer into a notebook

If you are caught using the "scrap of paper" technique, your improperly recorded data may be confiscated by your TA



Need to make the data available

Need to be able to find it

But how to expose it?

"First, they do an on-line search."

First, they do an online search

Jeremy G. Frey
University of Southampton

COSHH

Leverage off things we already have to do – "We have a cunning plan"

COSHH ASSESSMENT FORM Record No.

SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD
Water	liquid	1000ml	None
Dextrose	Solid	<20 g	possible irritation to eyes and skin
Caffeine	Solid (tea)	<1g	Harmful if swallowed, induce vomiting.
Milk	liquid	<100ml	No particular hazards

NATURE OF PROCESS
liquid extraction of caffeine, followed by combination with dextrose to produce a sweet drink

Is there a less hazardous substance? No
If so, why not use it?

CONTROL MEASURES REQUIRED No specific measure required
(Local exhaust ventilation, personal protection, etc.)

The fully semantic ELN - everything is linked!

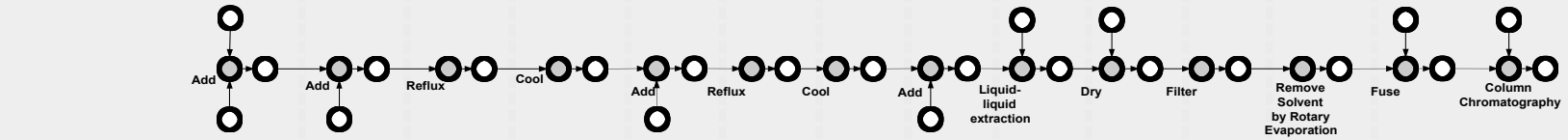
Jeremy G. Frey
University of Southampton

TO DO LIST

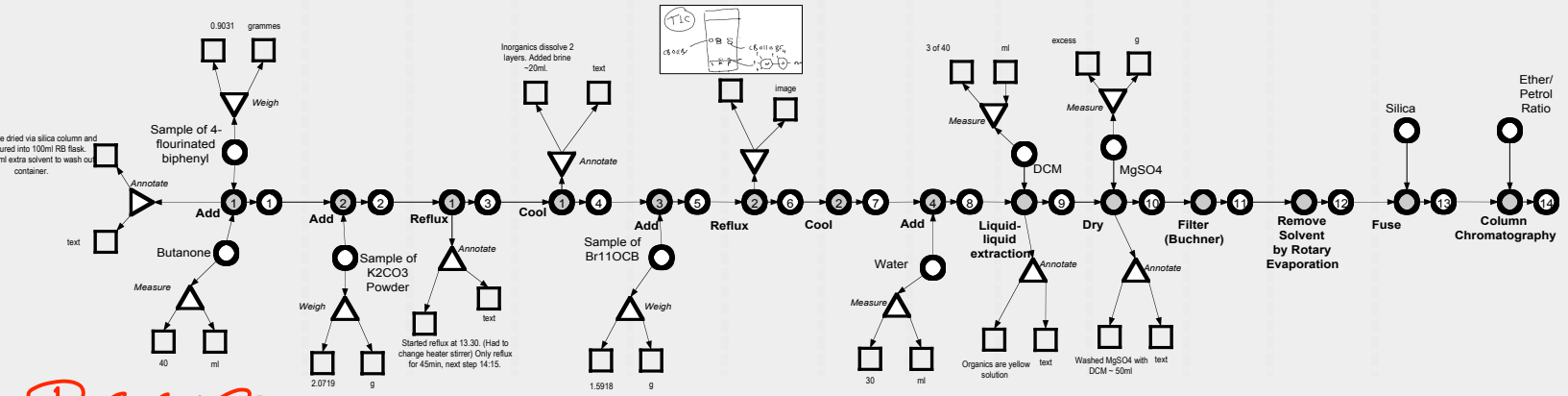
Ingredient List

Fluorinated biphenyl	0.9 g
Br11OCB	1.59 g
Potassium Carbonate	2.07 g
Butanone	40 ml

Dissolve 4-flourinated biphenyl in butanone | Add K2CO3 powder | Heat at reflux for 1.5 hours | Cool and add Br11OCB | Heat at reflux until completion | Cool and add water (30ml) | Extract with DCM (3x40ml) | Combine organics, dry over MgSO4 & filter | Remove solvent in vacuo | Fuse compound to silica & column in ether/petrol



PLAN



RECORD

Key

Process	○
Input	○
Literal	□
Observation	▽

Observation Types

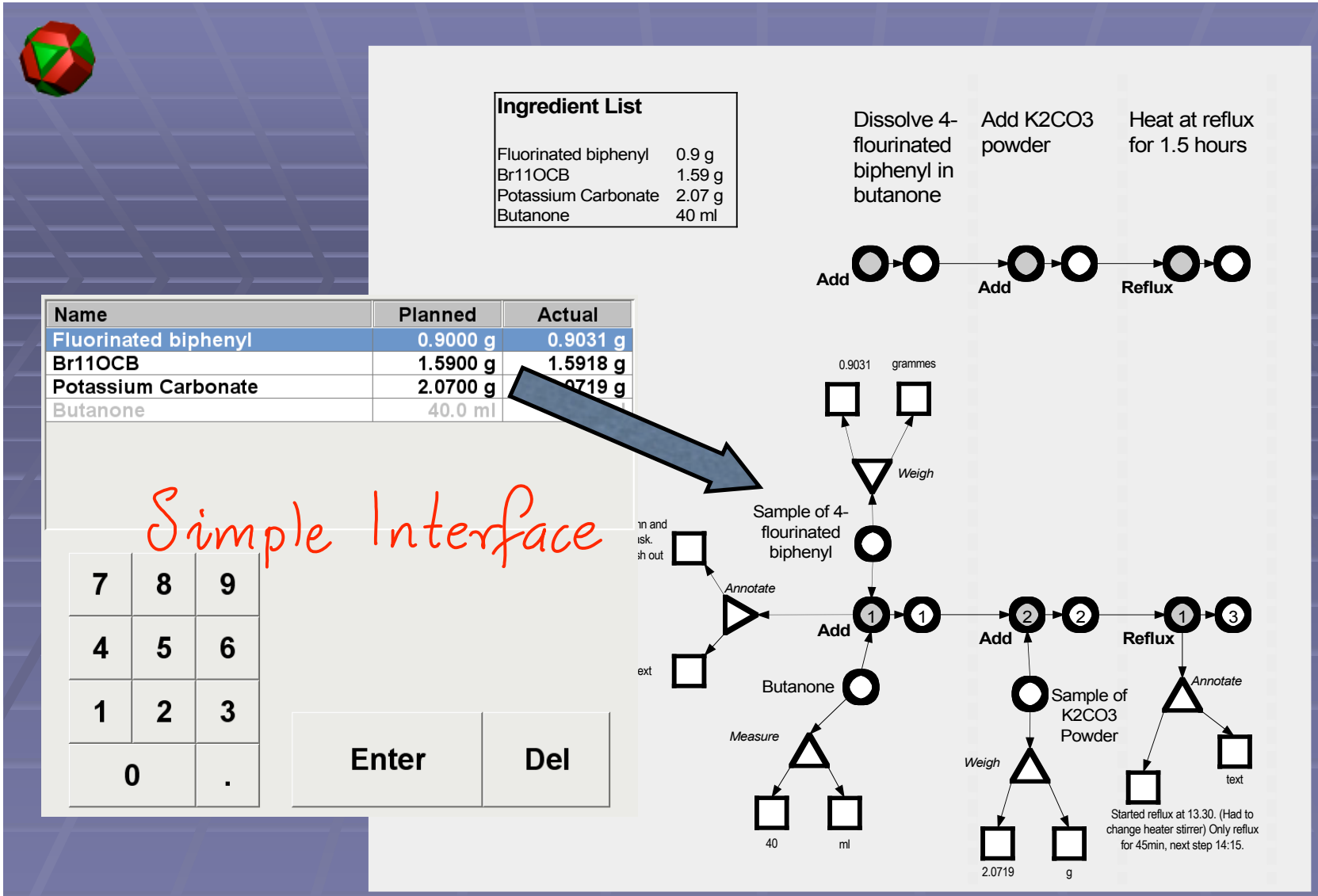
- weight - grammes
- measure - ml, drops
- annotate - text
- temperature - K, °C

Future Questions

- Whether to have many subclasses of processes or fewer with annotations
- How to depict destructive processes
- How to depict taking lots of samples
- What is the observation/process boundary? e.g. MRI scan

Combechem

30 January 2004
gvh, hrm, gms



Smart Tea Project - User Centred Design, Design by Analogy to ensure the correct information is captured simply and easily.

Jeremy G. Frey
University of Southampton

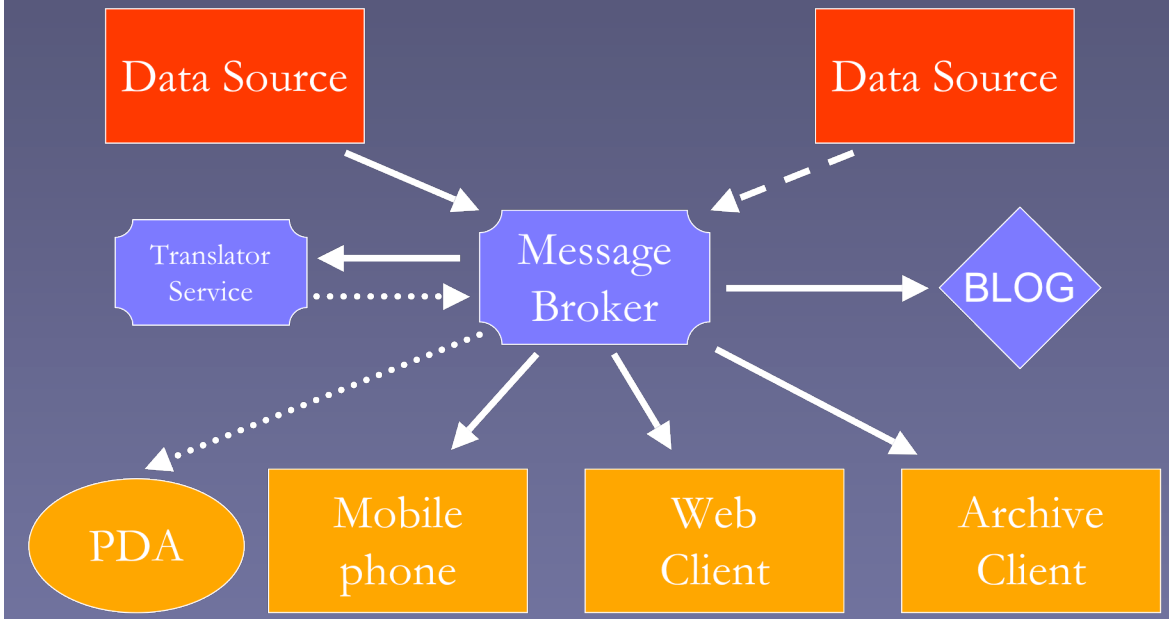
But what about the laboratory environment?

"I just realized, Howard, that everything in this apartment is more sophisticated than we are"

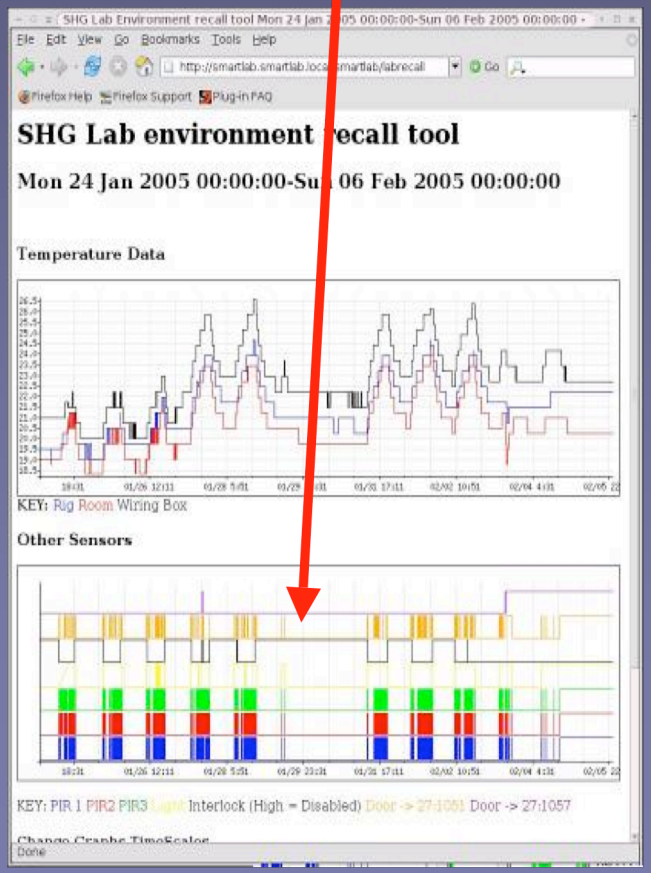
From *The New Yorker Book of Technology Cartoons.*

Jeremy G. Frey
University of Southampton

Pub-Sub systems provide the flexible & extensible approach to distribution of real time laboratory monitoring & archiving



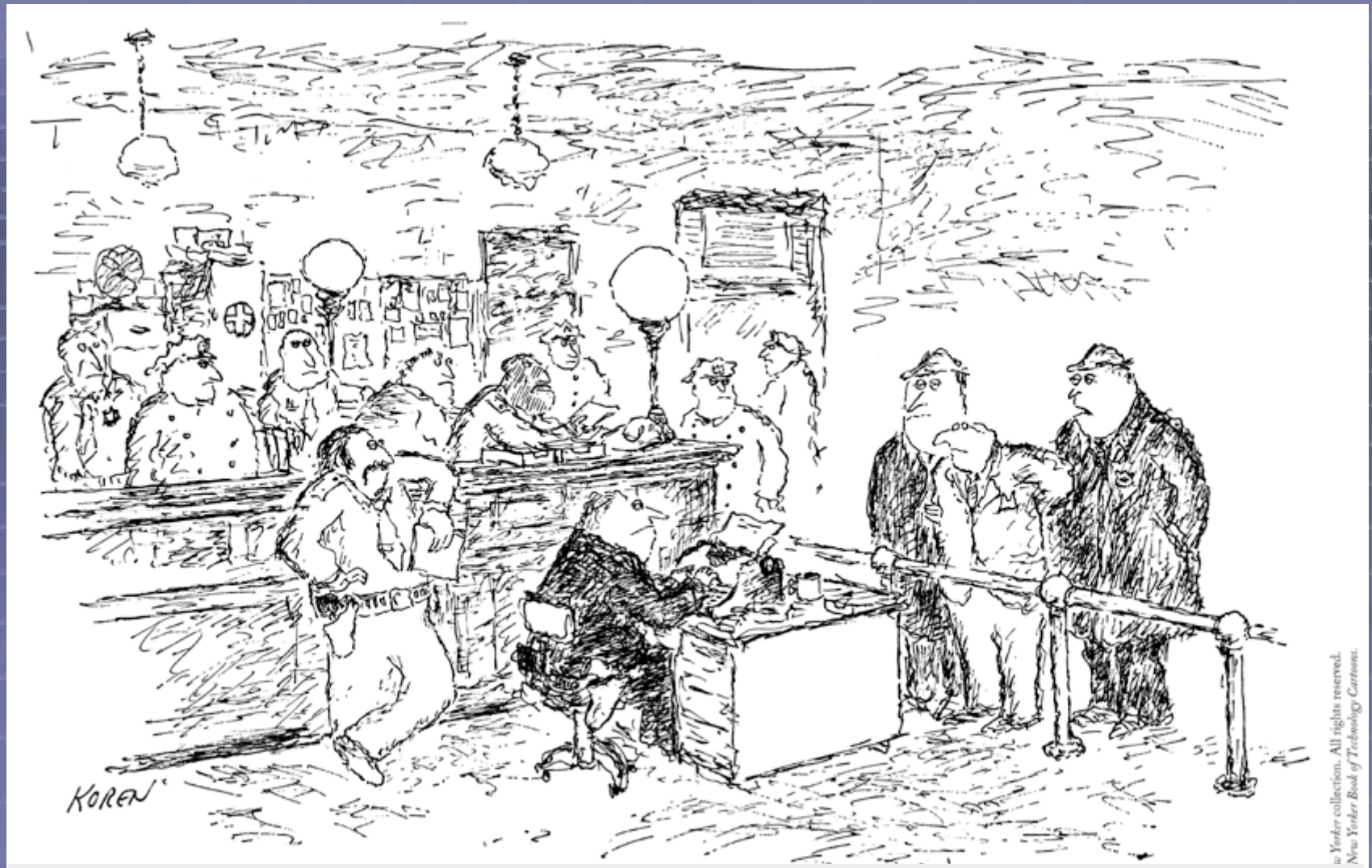
Air Conditioning failed



Smart Laboratory Spaces

Plans

- Plans in advance are useful
- This is the way things are supposed to be done
- The Plan provides a digital context so increases the value of planning
- Key to our ‘Smart Lab’ approach….
- But is it the best way?



He is charged with expressing contempt for meta-data

Jeremy G. Frey
University of Southampton

Laboratory “Blogs”

- Explore what is needed for a Blog to be the heart of an ELN
- Encourage and facilitate collaboration
- Need a data repository behind the Blog
  - R4L
  - E-Bank
- Building a VRE?

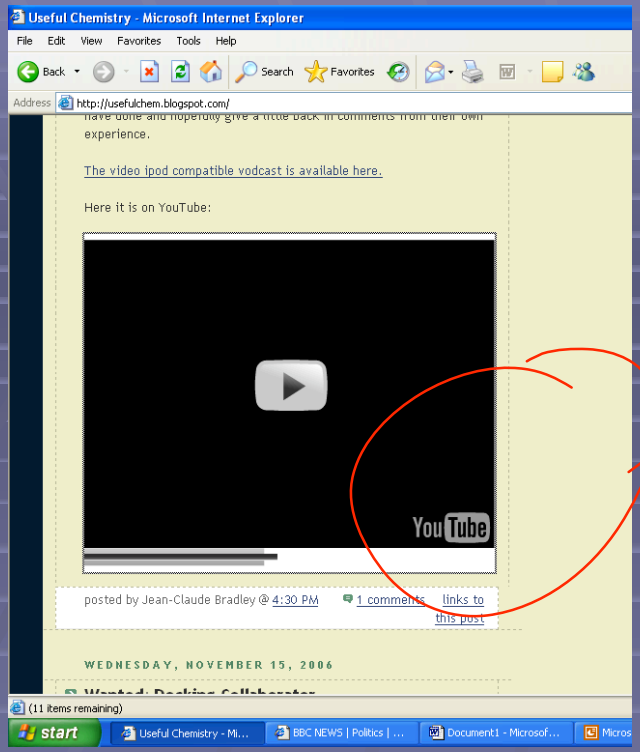
Jeremy G. Frey
University of Southampton

The 'Scientific Blog' is being tried in an attempt to combine laboratory notebooks and publication

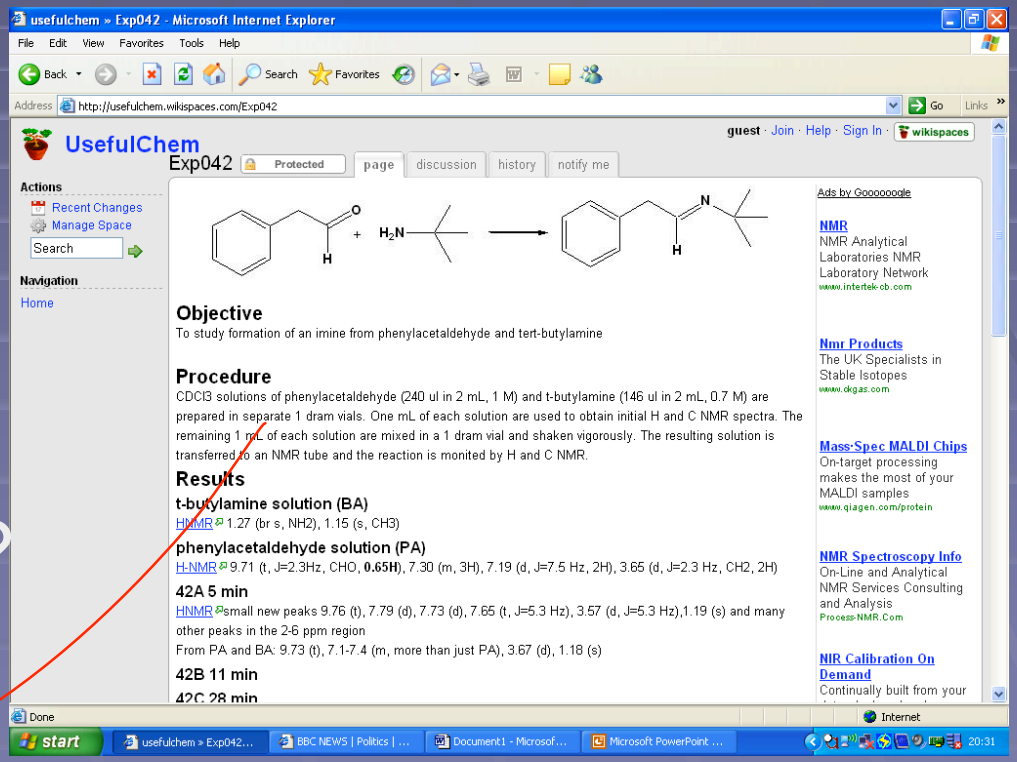
Public

Attribution

Immediate



Note the use of "YouTube"



An experiment that failed… Publishable? Useful?

Jeremy G. Frey
University of Southampton

Southampton Experiment Blogs

- Example from a Bio-Oganic Laboratory
  - Student (Jenny Hale)
    - Based in Southampton
  - Supervisor (Cameron Neylon)
    - Southampton only 1/3 time, RAL 2/3 time

Transformation of plasmid JRH4712/66 into BW25141 by electroporation

11th December 2006 @ 14:31

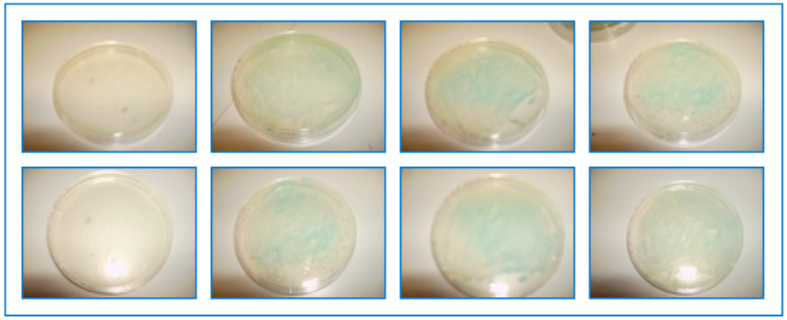
Transformations were set up according to the following protocol:
LB Ampicillin arabinose plates and SOC medium were warmed to 37 °C briefly before the arabinose plates were spread with X-glu (80 µL, 1:1 X-glu and LB) and allowed to continue warming.

BW25141 cells, plasmid JRH4712/66, p042, and electroporator cuvettes were cooled on ice. Items were added to the cuvettes as follows

-	1	+ve ctrl	-ve ctrl
BW25141	40 µL	40 µL	40 µL
plasmid 4712/66	4 µL	0 µL	0 µL
p042	0 µL	4 µL	0 µL

Cuvettes were electroporated at 1.75 kV, immediately had SOC medium (950 µL) added and the transformant transferred to eppendorf. The transformants were incubated at 37 °C for one hour with shaking. The transformants were diluted 1 in 20 with LB and 100 µL added to LB amp arabinose plates and incubated at 37 °C overnight.

Data



Jennifer Hale | Beta-glucuronidase | Comments (3)

Archives

January 2007 (24)
December 2006 (11)
November 2006 (5)

Sections

beta-galactosidase preparation and assays (18)
Beta-glucuronidase (18)
Data (Formatting) (1)
Software discussions (2)
Starting materials and reagents (1)

Lab Book Ref

JRH4712-63 (1)
JRH4712-64 (2)
JRH4712-66 (1)
jrh4712-76 (1)
jrh4712-77 (1)

Test digestions to check the activity of two batches of EcoRI and NcoI

22nd January 2007 @ 11:57

Lab Book Ref: jrh4712-89
Sample Parent: jrh4712-80_blue
Sample Parent2: jrh4712-80_white
Digestions were set up as follows:

-	1	2	3	4	5	6	7	8	9	10	11
4712/80 blue	8 µL	-	-	8	-	-	-	8 µL	-	-	-
4712/80 white	-	8 µL	-	-	8 µL	-	-	-	8 µL	-	-
p042	-	-	5 µL	-	-	5 µL	5 µL	-	-	5 µL	5 µL
water	7.5 µL	7.5 µL	10.5 µL	7.5 µL	7.5 µL	10.5 µL	10 µL	7.5 µL	7.5 µL	10.5 µL	10 µL
*Eco*RI buffer	2 µL	2 µL	2 µL	-	-	-	2 µL	2 µL	2 µL	2 µL	2 µL
NEB buffer 4	-	-	-	2 µL	2 µL	2 µL	-	-	-	-	-
BSA	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL
*Eco*RI (a)	0.5 µL	0.5 µL	0.5 µL	-	-	-	0.5 µL	-	-	-	-
*Nco*I	-	-	-	0.5 µL	0.5 µL	0.5 µL	0.5 µL	-	-	-	0.5 µL
*Eco*RI (b)	-	-	-	-	-	-	-	0.5 µL	0.5 µL	0.5 µL	0.5 µL

*Eco*RI (a) assay date 2/05
*Eco*RI (b) assay date 7/05

Digestions were incubated in a waterbath at 37 °C for 3 hours.

Archives

January 2007 (24)
December 2006 (11)
November 2006 (5)

Sections

beta-galactosidase preparation and assays (18)
Beta-glucuronidase (18)
Data (Formatting) (1)
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Starting materials and reagents (1)

Lab Book Ref

JRH4712-63 (1)
JRH4712-64 (2)
JRH4712-66 (1)
jrh4712-76 (1)
jrh4712-77 (1)
jrh4712-78 (1)
jrh4712-80 (1)
jrh4712-81 (1)
jrh4712-83 (1)
jrh4712-82 (1)
jrh4712-84 (1)
jrh4712-85 (1)
4712-88 (1)
jrh4712-89 (1)
4712-86 (1)
jrh4712-87 (1)
4712-90a (1)

Product

jrh4712-74 (1)
jrh4712-76 (1)
jrh4712-76a (1)

Mutagenesis of plasmid p042 via Taq and GenemorphI

9th January 2007 @ 14:34

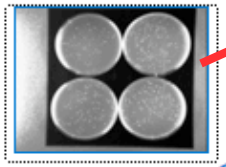
Lab Book Ref: jrh4712-78

Mutagenic PCR reactions were set up according to the following:

-	Taq	GenemorphI	+ve ctrl	-ve ctrl
p042	2.5 µL	1 µL	5 µL	0 µL
Water	10 µL	38 µL	20.5 µL	25.5 µL
5 x GoTaq buffer	10 µL	-	10 µL	10 µL
mutazyme buffer	-	5 µL	-	-
Ordinary dNTPs	-	-	5 µL	5 µL
mutagenic dNTPs	5 µL	-	-	-
Mutazyme dNTP mix	-	1 µL	-	-
MgCl2	2.5 µL	-	3.5 µL	3.5 µL
MnCl2	12.5 µL	-	-	-
Primer fwd	2.5 µL	2 µL	2.5 µL	2.5 µL
Primer rev	2.5 µL	2 µL	2.5 µL	2.5 µL
GoTaq*	1 µL	-	1 µL	1 µL
Mutazyme	-	1 µL	-	-

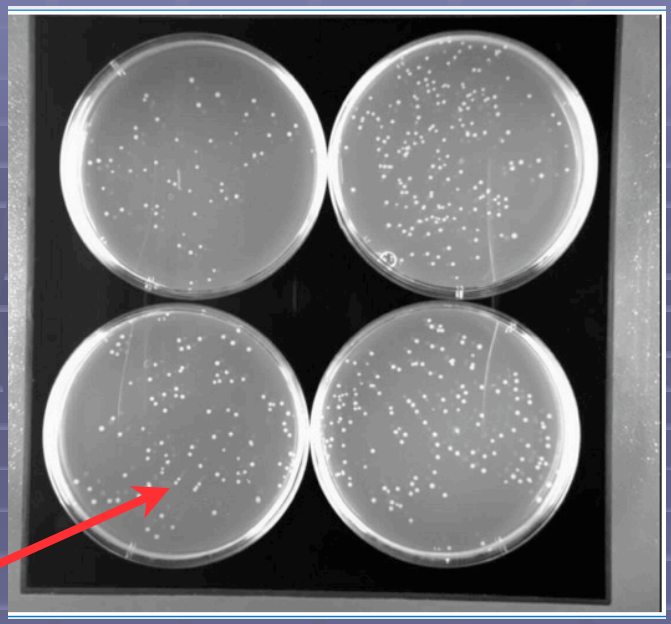
*GoTaq=1 µL stock + 3 µL water.

The reactions were run on program MUTAGBG for 30 cycles. 5 µL product was run on a 1% normal agarose analytical gel. Taq mutagenesis had failed, Genemorph and +ve ctrl had worked. -ve control was correct.



Jennifer Hale | Beta-glucuronidase | Comments (3)

<< Previous Page Next Page >>



Re: PCR of beta-galactosidase third attempt by Jennifer Hale

14th December 2006 @ 11:10

Unfortunately the purification appears not to have gone well. Though I also can't get any consistency from the figures given by the nano-drop. These are the results I got:

-	reading 1	reading 2	reading 3	reading 4	reading 5	reading 6	average
PCR product before*	282.3 ng/µL	283.4 ng/µL	281.1 ng/µL	N/A	N/A	N/A	282.3 ng/µL
PCR product after*	7.8 ng/µL	12.9 ng/µL	17.6 ng/µL	85.4 ng/µL	22.4 ng/µL	12.8 ng/µL	?

*Both reactions combined together after PCR

I'm going to do another PCR again. That step is working really well. I'm just not sure what to do about purifying it. The only other thing I can try is eluting in TE buffer rather than water (which it says you can also elute into)
In this purification I used preheated water and followed the instructions closely. Perhaps the DNA will elute into TE more effectively.

Re: PCR of beta-galactosidase third attempt by David Neylon

14th December 2006 @ 18:32

I would definitely compare these on a gel so as to see whether it is just the nanodrop that is the problem. It might help also if you are explicit about how much solution you are trying to purifiy and what the final volume is.

jrh4712-80_blue (2)
4712-86 (1)
4712-84_beta-gal (1)
4712-80_blue (1)
4712-88 (1)

Sample Parent2

jrh4712-80_blue (1)
jrh4712-80_white (2)
4712-84_pBad (1)
4712-80_white (1)

Sample Parent 3

4712-74 (1)

Search

Find

Links

Admin

New Post

Live Copy

Re: Software development by Jennifer Hale
1st December 2006 @ 15:03

I'm not sure that I trust this thing. Just now there was an error message saying there were syntax errors in the mySQL. my post had appeared twice and my comment had disappeared. I close the window and then log back in and it all seems to be okay: the post appears once and my comment has reappeared but the post I wrote in response to the posts apparently disappearing and doubling up has disappeared.

Re: Software development by Andrew Milsted
1st December 2006 @ 17:18

I am working on the session problem, I have looked at the long list and most of the points are on my todo list. I will let you know when thing become availble. If you are writing long posts (i know this sounds crazy) but use word and copy and paste into the blog, once i have fixed the sessions this won't be needed.

Re: Software development by Jennifer Hale
5th December 2006 @ 11:19

My gel pictures when seen in close up are awful quality - very pixellated. It doesn't show a clear picture at all. Should I try saving the files as a different file type as they are currently a jpeg?
The thing I don't understand the most though is that if I click on the file on my computer and it opens up in photo editor or viewer or whatever it is, the picture is fine even on a large scale - really clear.

Instrument Blog

Login more blogs

MQTT Lego Microscope

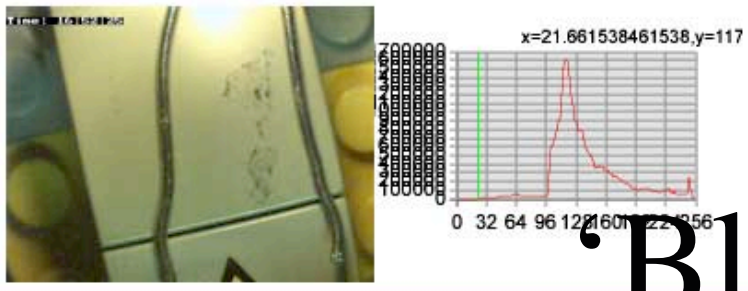
A highly advanced remote control microscope.

Data Collection

15th September 2006 @ 16:52

A data collection was made by Andrew Milsted (ajm3) with sample description: Paper Clip

Data



ajm3 | Data Collection | Comments (0)

Archives

September 2006 (2)

Sections

Data Collection (2)

Search

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Links

‘Blog-jects’

Jeremy G. Frey
University of Southampton

Pub-Sub

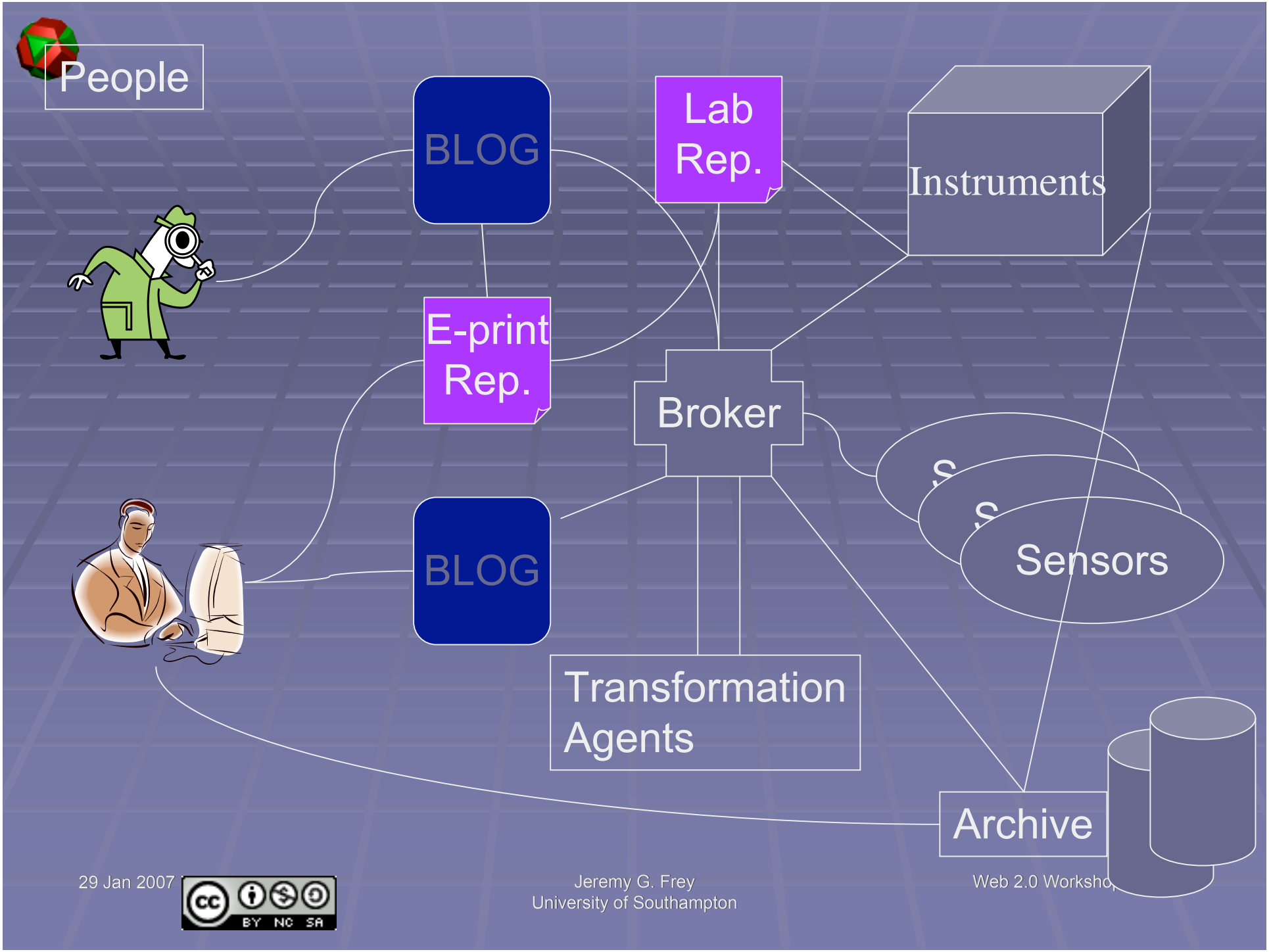
- Pub Sub & Data Brokers
  - Important way to include laboratory environmental & people data in a flexible manner
  - Backed by archive database service
  - Correlate with experiments via time & place

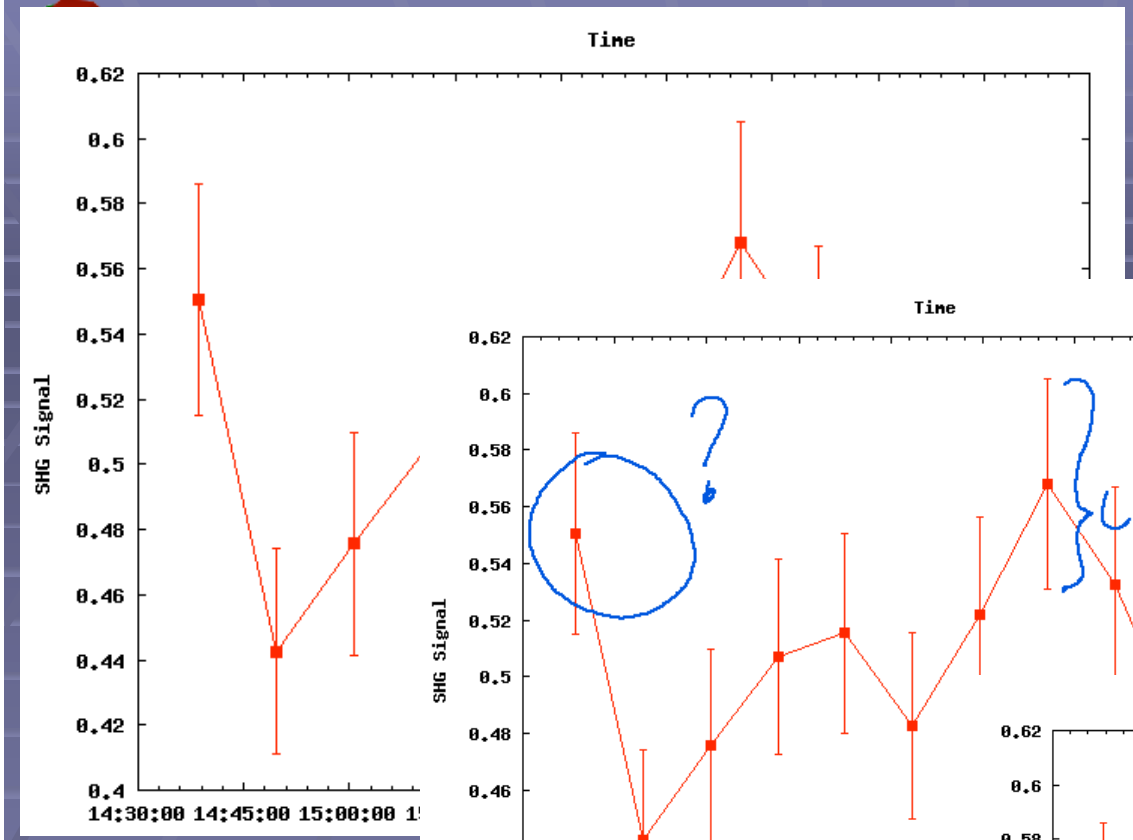
Jeremy G. Frey
University of Southampton

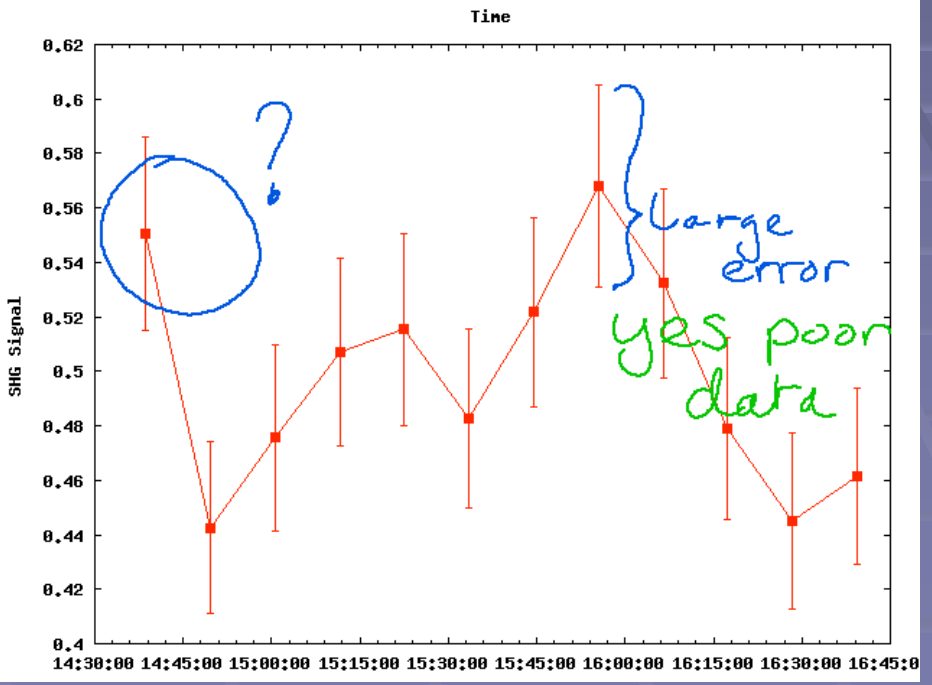
Blog-jects

- Equipment become first class members of the web
- Interacts well with Pub-Sub as items are attached to topics, topics relate the Bog items
- With automation this evolves to a two-way communication
- Live Copy essential

Jeremy G. Frey
University of Southampton


People
BLOG
Lab Rep.
Instruments
E-print Rep.
Broker
BLOG
Sensors
Transformation Agents
Archive





Comments and Annotation don't need to be just text. Chemists like to sketch!

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Validation

- Increasing the value of data
- How to bring all the necessary information together to enable appropriate validation
- Increasingly difficult & expensive to achieve
- Need provenance and context
- Essential step otherwise just a collection of items

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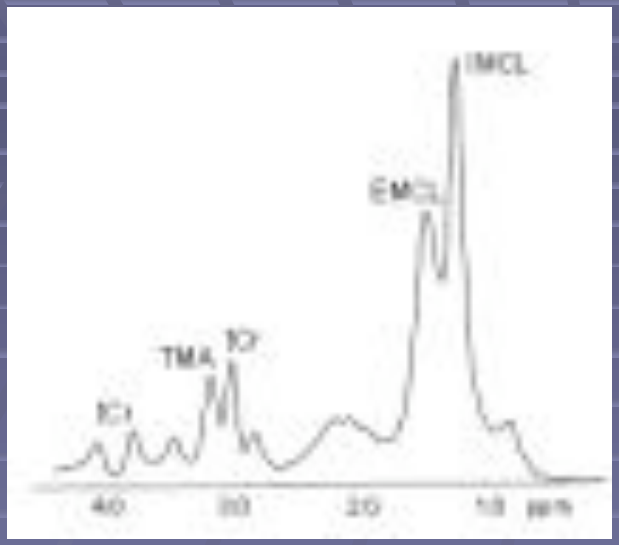
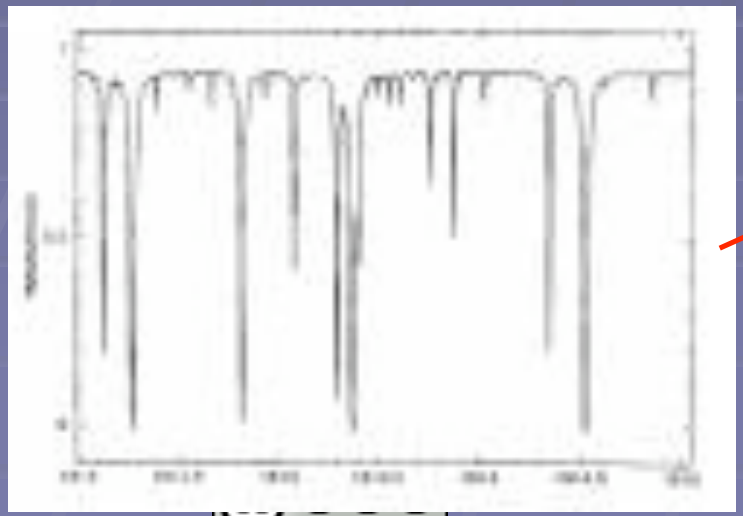
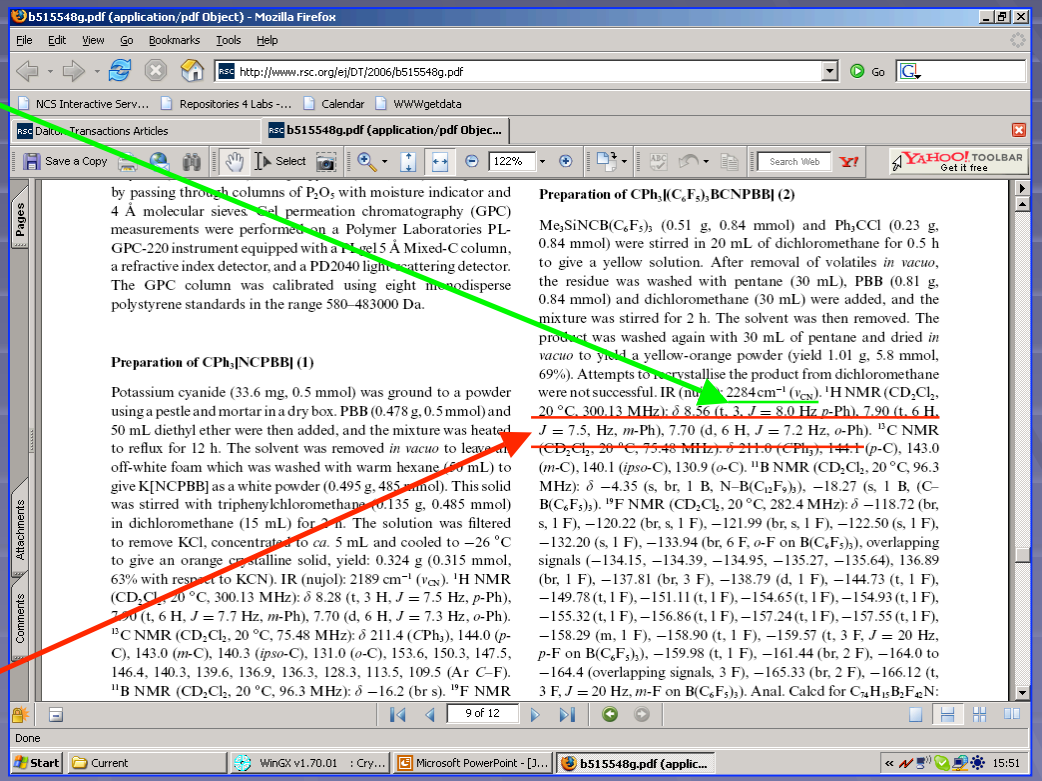
Why?
Publishing Data and Information Loss







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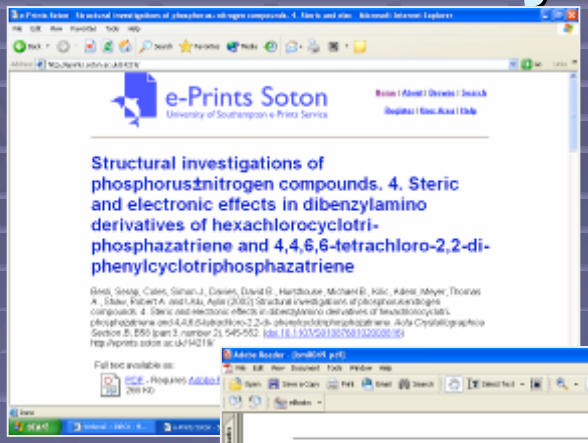
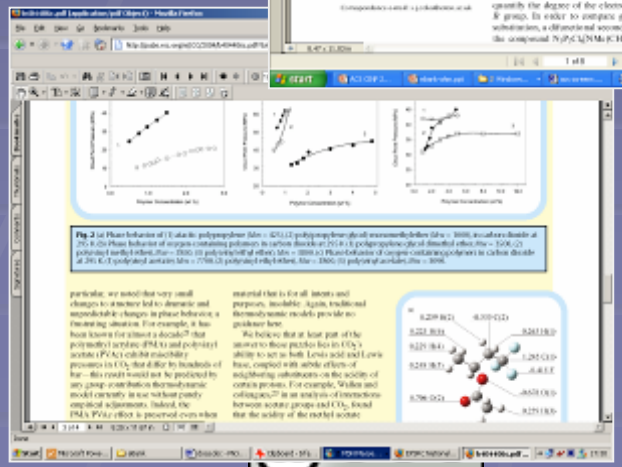
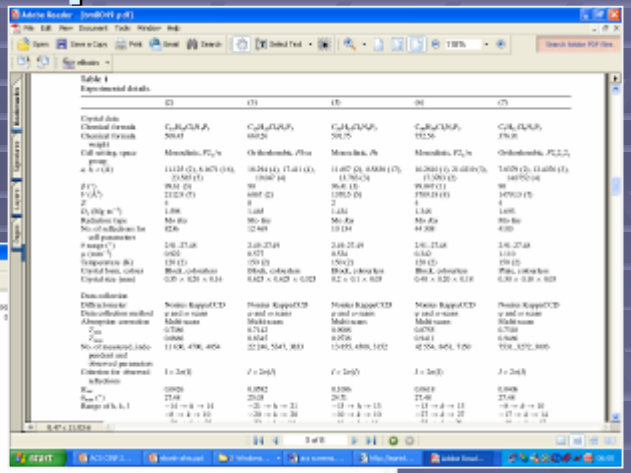
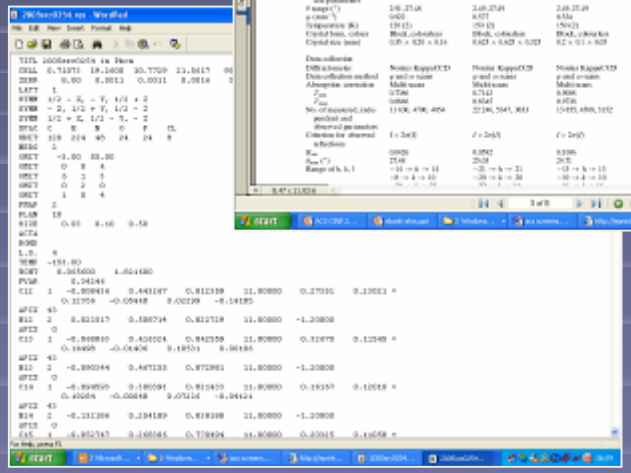
Separating Data from Interpretations: A crystallography example



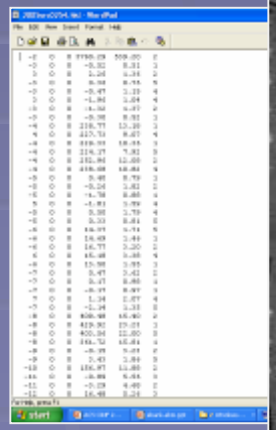


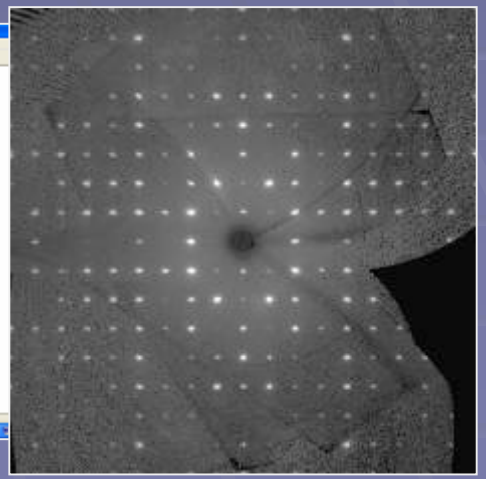
Intellect & Interpretation





Underlying data





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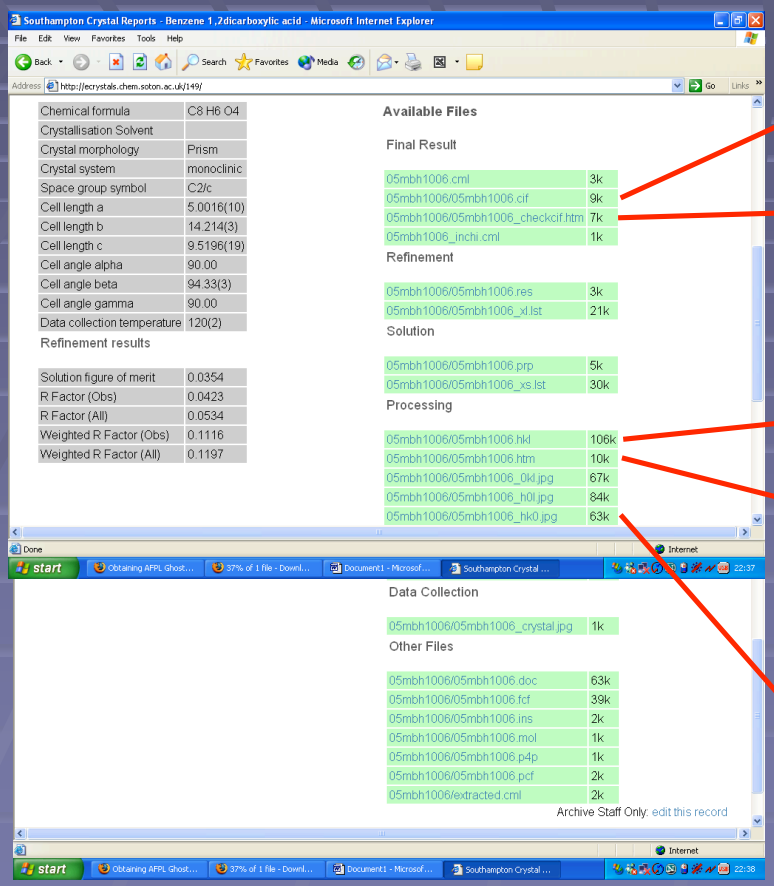
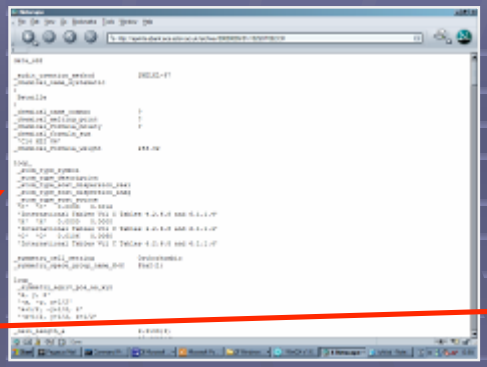
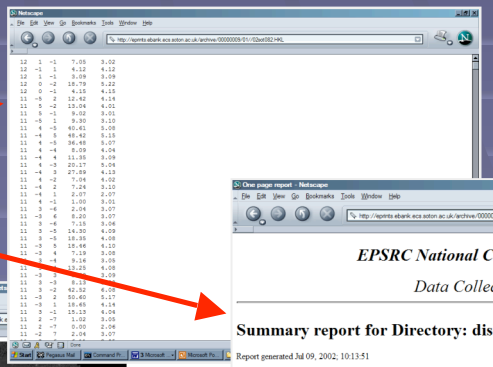
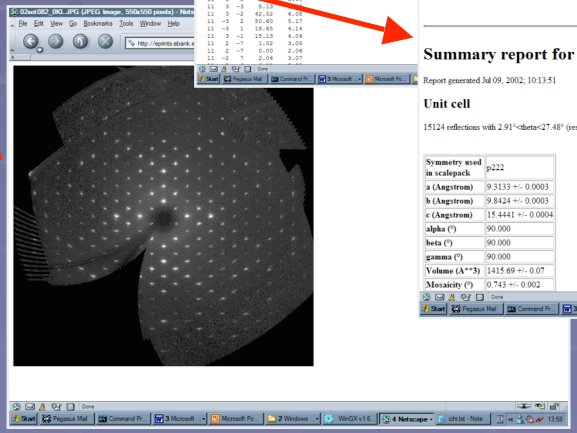
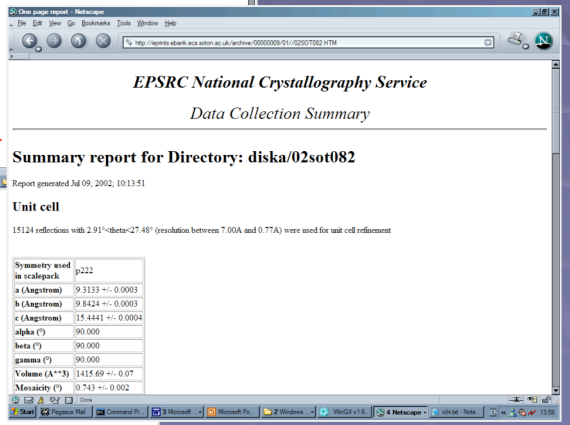
Access to ALL underlying data











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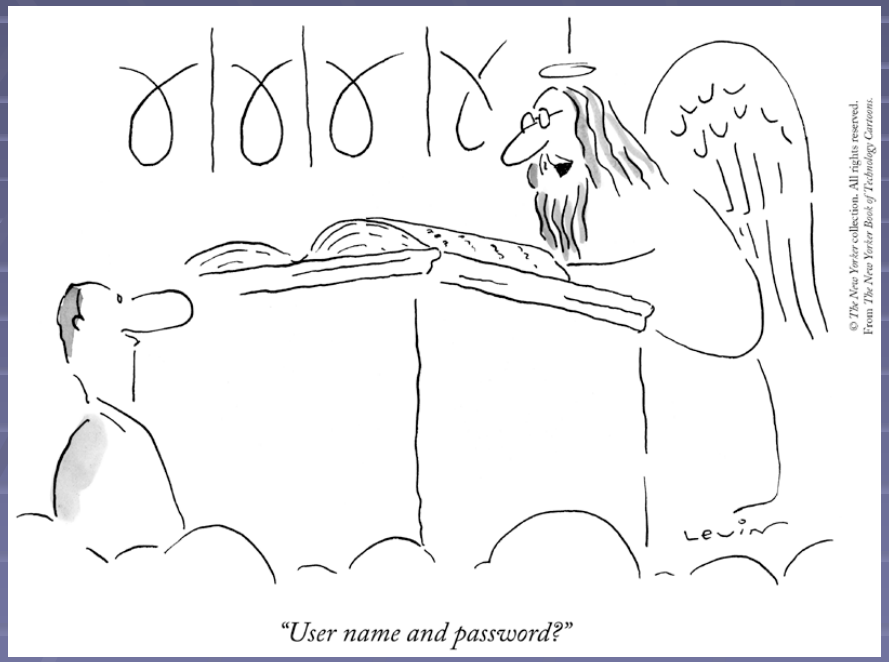
Wireless Technology



"User name and password?"

- Location independence? Is this always a good idea
- Library material can be brought to all places but knowledge & experience about the information available is more difficult

"User name and password?"
No! A library card won't do.

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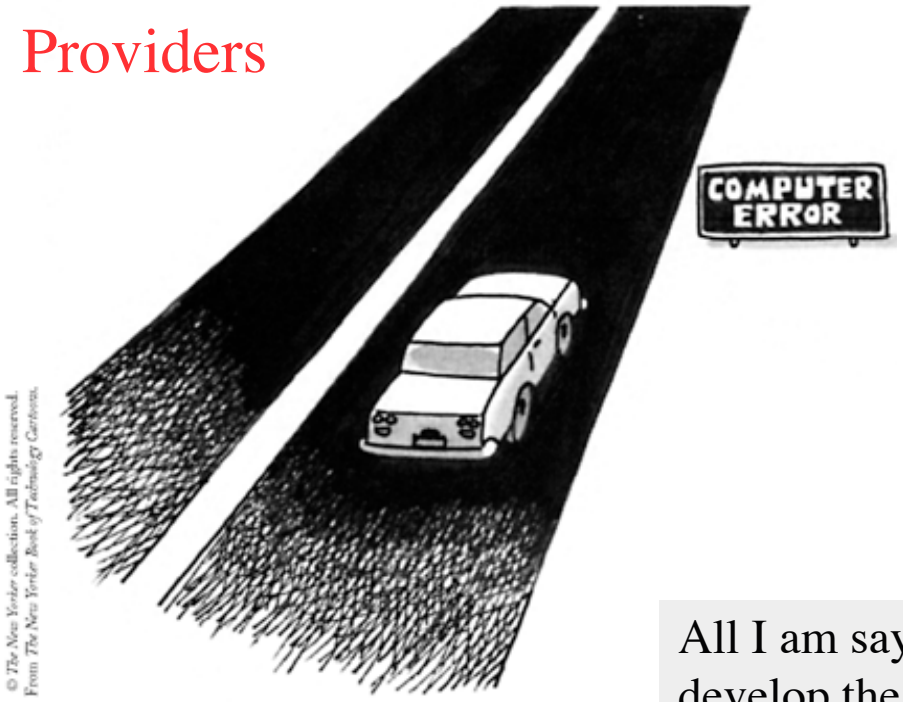
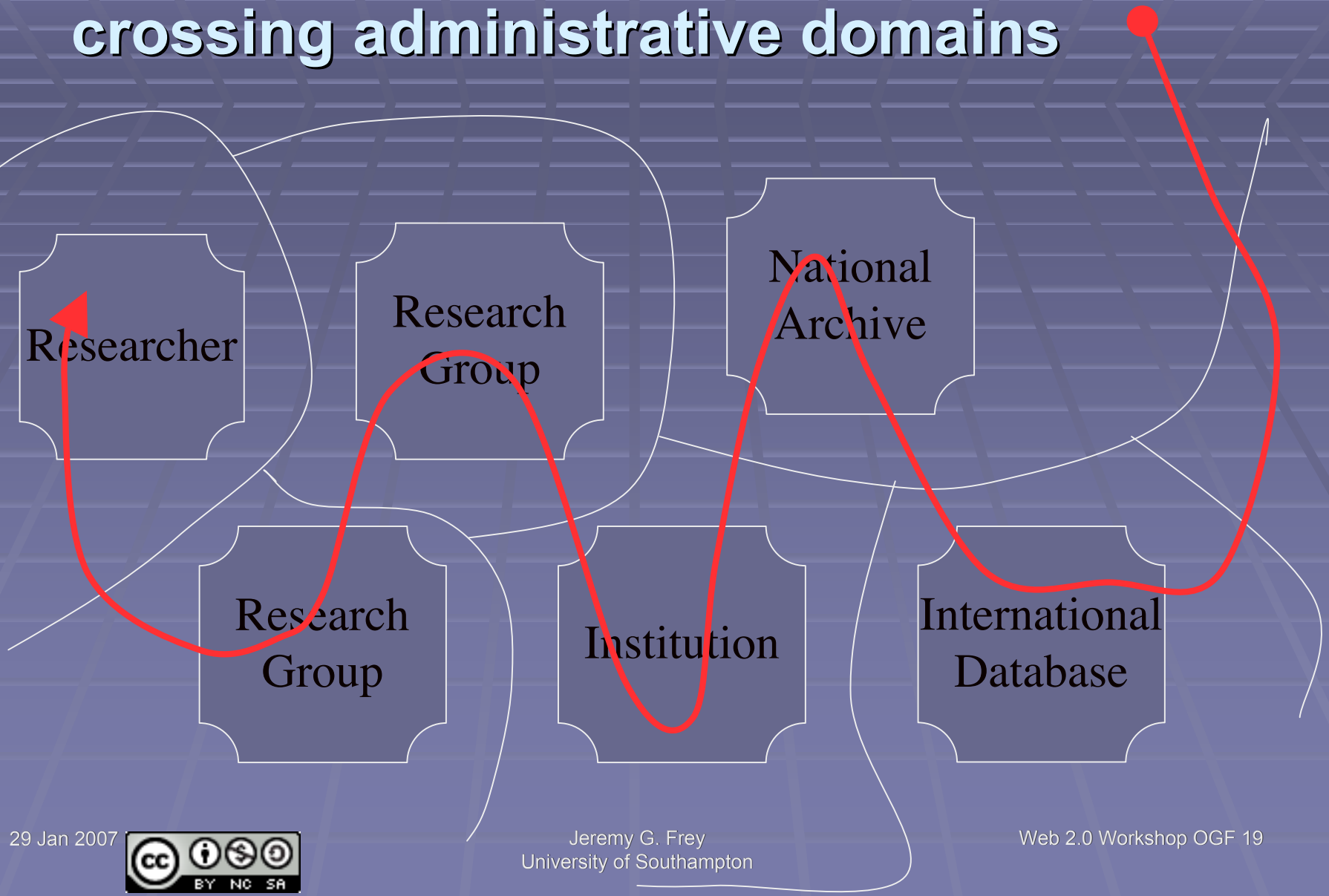
Information Consumers

Information Providers



All I am saying is that now is the time to develop the technology to deflect an asteroid

Access to information requires crossing administrative domains



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PEOPLE

- Southampton CHEMISTRY, ECS, MATHS,IT-INNOVATION
- BRISTOL
- UKOLN
- CCLRC
- INDIANA
- SYDNEY
- MANCHESTER

- Funding
- EPRSC e-Science & Chemistry Programmes
- JISC DTI

- See web site for full details and links
- www.combechem.org

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