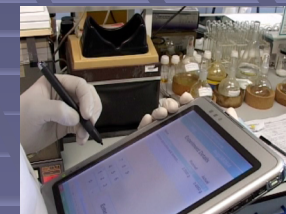
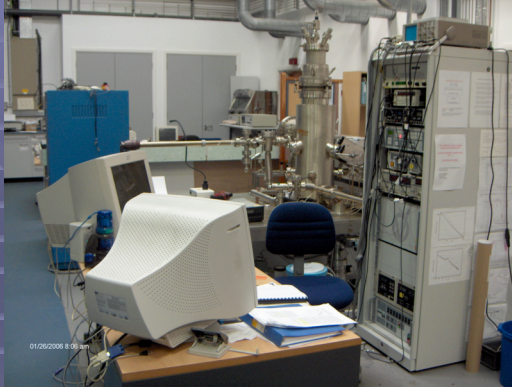


Smart Lab 2.5

The digital future of laboratory Chemistry

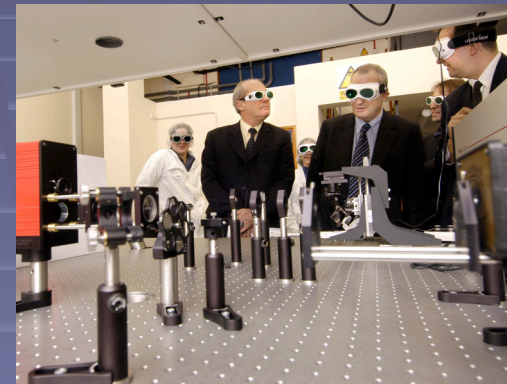
Jeremy G.Frey
School of Chemistry
University of Southampton, UK





Talk

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



29 Jan 2007



Jeremy G. Frey
University of Southampton

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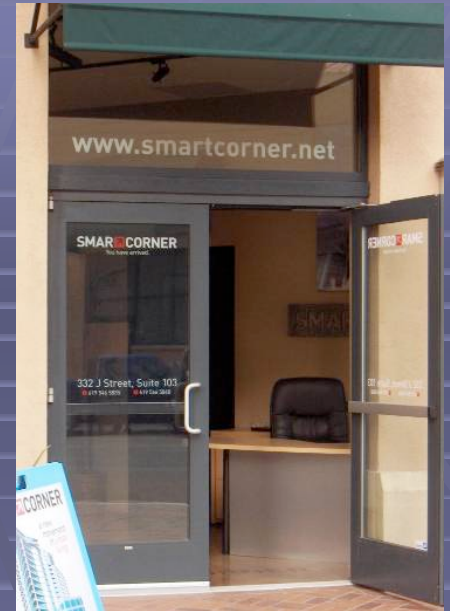


Research Space

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.....



29 Jan 2007



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?

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University of Southampton

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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



Combechem

Smart Lab

E-Malaria

R4L

Instruments on the Grid

e-Bank

Statistics

BioSimGrid



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

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

Typical Laboratory



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.

ChemLab

The Chemistry 3/5 & 6
Laboratories

- ▶ General Information
- ▶ Instruments & Techniques
- ▶ Chemistry 3/5 Experiments
- ▶ Chemistry 6 Experiments

DARTMOUTH COLLEGE

Permanent,
documented
and primary
record of
laboratory
observations

Safety

- [General Rules](#)
- [Safety Equipment](#)
- [Safety Hazards](#)
- [Emergency Procedures](#)

Resources

- [Applets](#)
- [General FAQ](#)
- [Uncertainty](#)
- [ChemLab Home](#)

[Info](#) | [Techniques](#) | [Chem 3/5](#) | [Chem 6](#)

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.

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 turn in your prelab problems from the manual for grading. 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



Jeremy G. Frey
University of Southampton

2.0 Workshop OGF 19



Need to make
the data
available

Need to be
able to find it

But how to
expose it?



First, they do an online search



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	Soln	<20g	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 (Local exhaust ventilation, personal protection, etc.) No specific measure required			



The fully semantic ELN - everything is linked!

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To Do List

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

Dissolve 4-fluorinated 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)

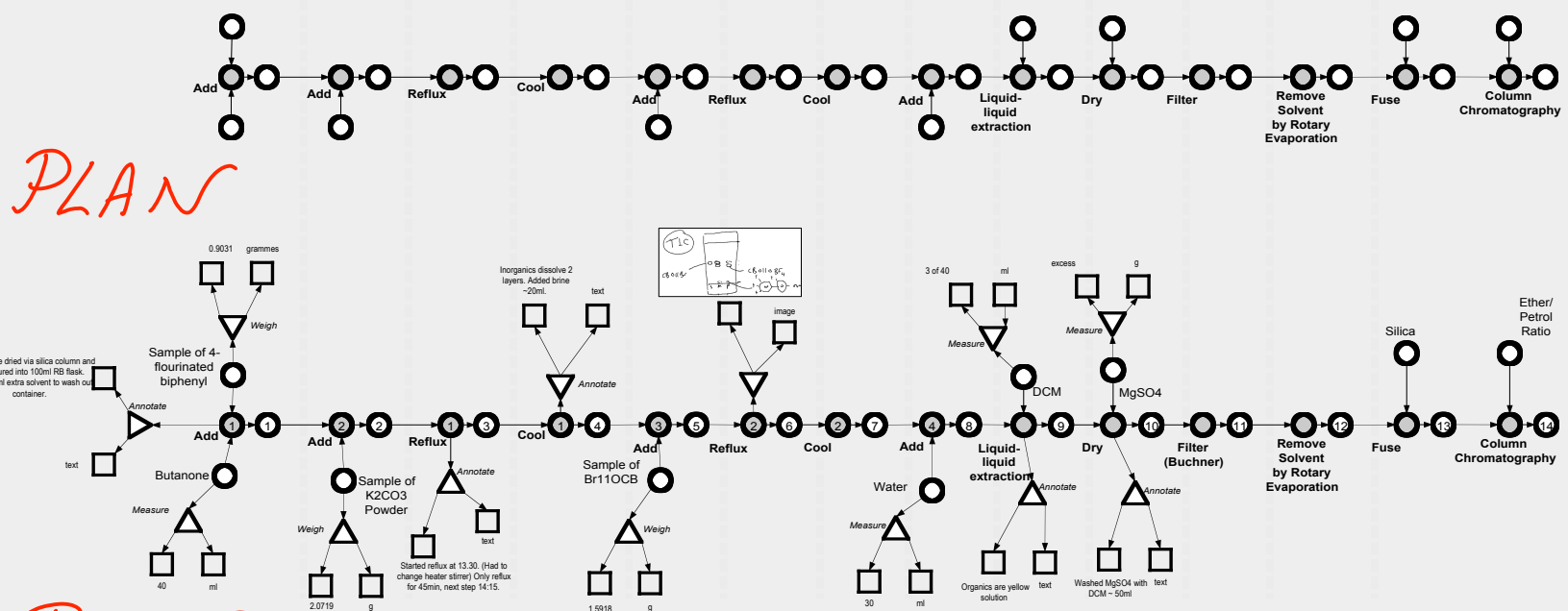
Combine organics, dry over MgSO₄ & filter

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



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



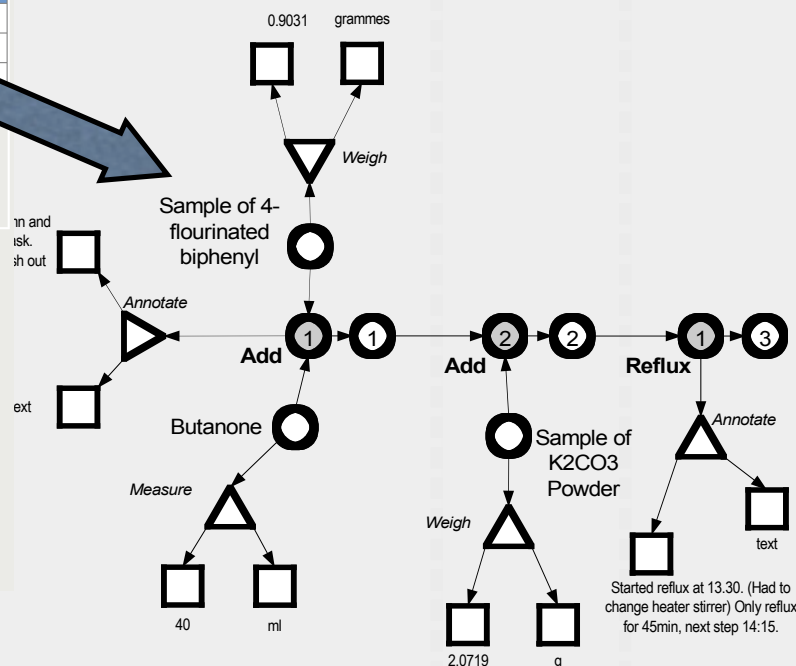
Name	Planned	Actual
Fluorinated biphenyl	0.9000 g	0.9031 g
Br11OCB	1.5900 g	1.5918 g
Potassium Carbonate	2.0700 g	2.0719 g
Butanone	40.0 ml	

Simple Interface

7	8	9
4	5	6
1	2	3
0	.	

Enter

Del



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

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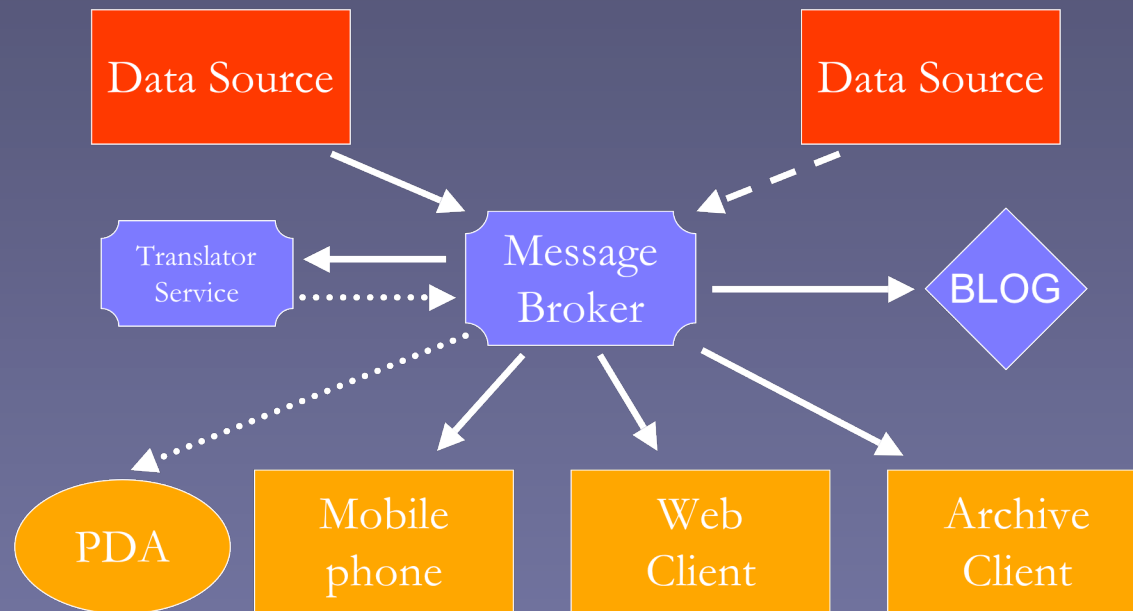
But what
about the
laboratory
environment?



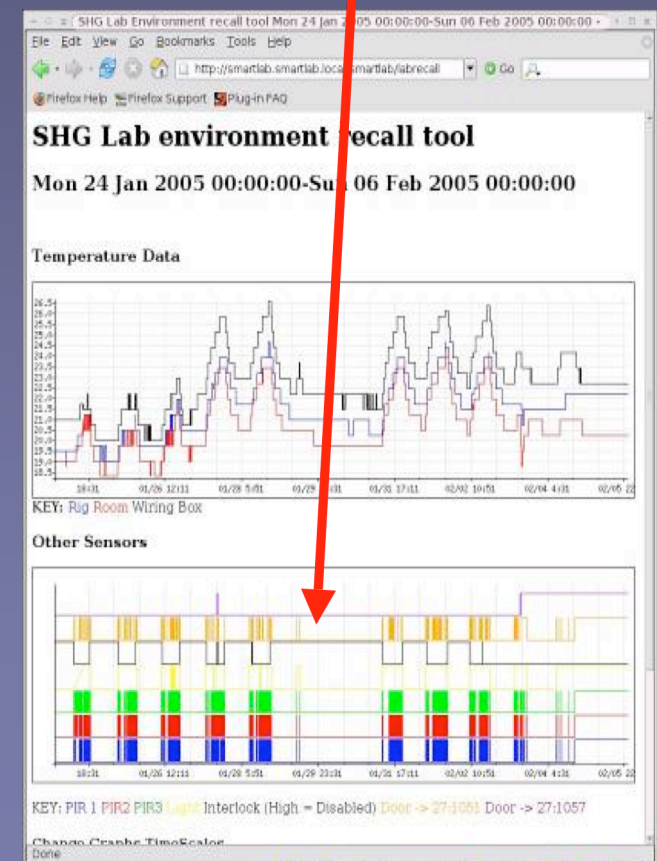
**"I just realized, Howard, that everything
in this apartment is more sophisticated
than we are"**

© 2007 New Yorker collection. All rights reserved.
From *The New Yorker Book of Technology Cartoons*.

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



Air Conditioning failed

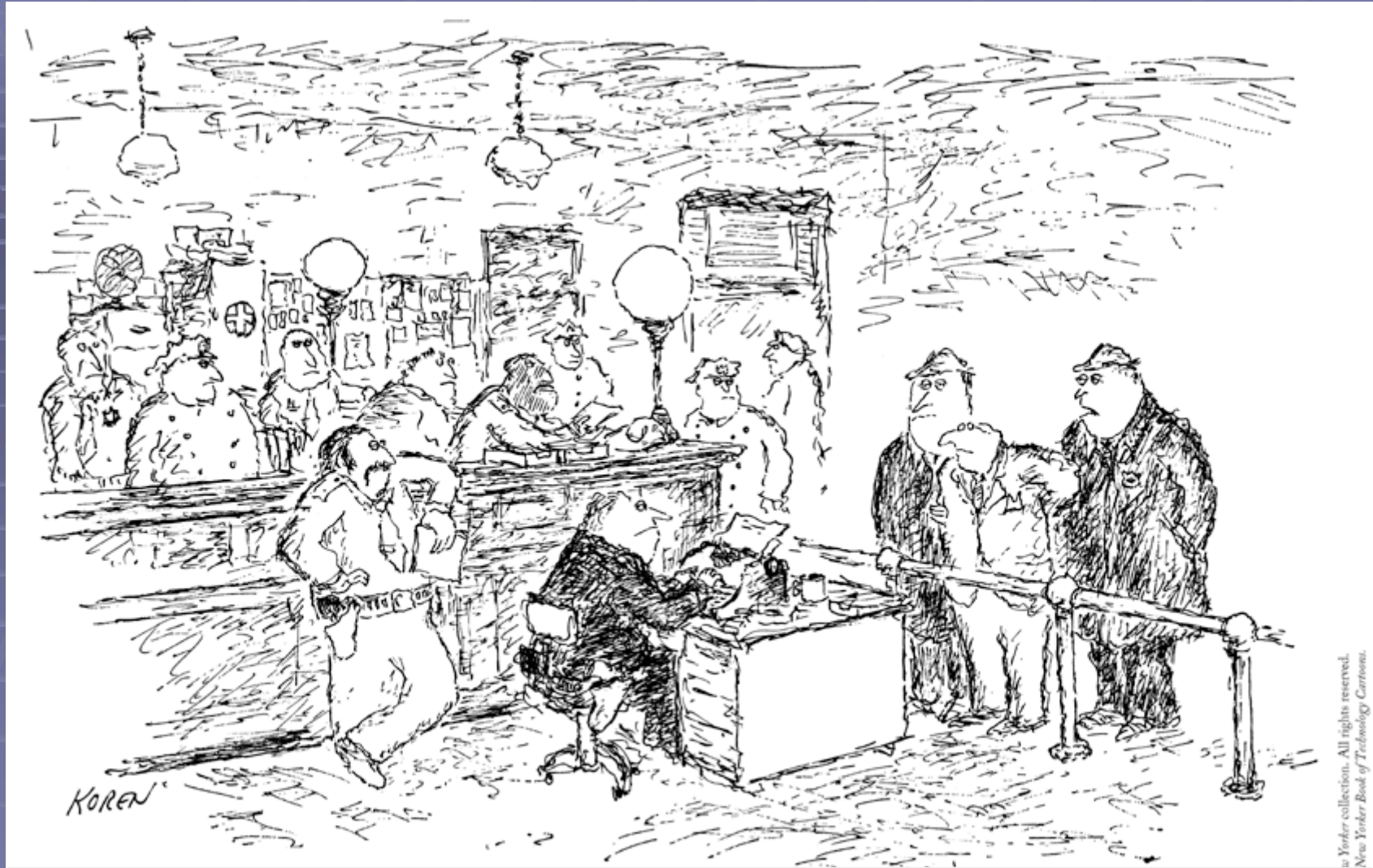


Smart Laboratory Spaces



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

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University of Southampton

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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?



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

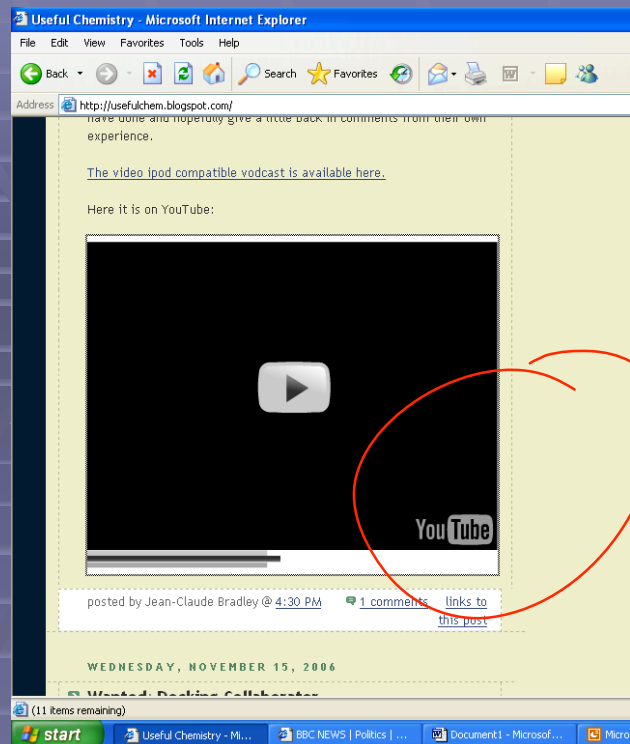
Public

Attribution

Immediate

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Workshop OGF 19



Note the use of
"YouTube"

An experiment that
failed... Publishable?
Useful?

UsefulChem
Exp042

Objective
To study formation of an imine from phenylacetaldehyde and tert-butylamine

Procedure
CDCl₃ solutions of phenylacetaldehyde (240 μ l in 2 mL, 1 M) and t-butylamine (146 μ l in 2 mL, 0.7 M) are prepared in separate 1 dram vials. One mL of each solution are used to obtain initial H and C NMR spectra. The remaining 1 mL of each solution are mixed in a 1 dram vial and shaken vigorously. The resulting solution is transferred to an NMR tube and the reaction is monitored by H and C NMR.

Results
t-butylamine solution (BA)
H-NMR δ 1.27 (br s, NH₂), 1.15 (s, CH₃)
phenylacetaldehyde solution (PA)
H-NMR δ 9.71 (t, J=2.3 Hz, CHO, 0.65H), 7.30 (m, 3H), 7.19 (d, J=7.5 Hz, 2H), 3.65 (d, J=2.3 Hz, CH₂, 2H)
42A 5 min
H-NMR δ small new peaks 9.76 (t), 7.79 (d), 7.73 (d), 7.65 (t, J=5.3 Hz), 3.57 (d, J=5.3 Hz), 1.19 (s) and many other peaks in the 2-6 ppm region
From PA and BA: 9.73 (t), 7.1-7.4 (m, more than just PA), 3.67 (d), 1.18 (s)
42B 11 min
42C 28 min

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Southampton Experiment Blogs

- Example from a Bio-Organic 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

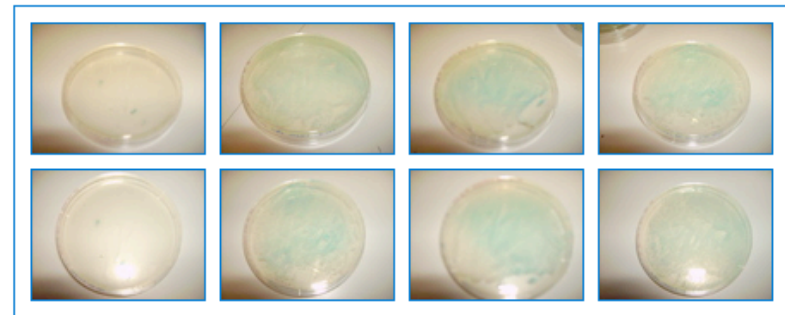
Transformations were set up according to the following protocol: LB Ampicillin arabinose plates and SOC medium were warmed to 37 °C briefly before the arabinose plates were spread with X-glu (80 µL, 1:1 X-glu and LB) and allowed to continue warming.

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

[JR4712-63 \(1\)](#)
[JR4712-64 \(2\)](#)
[JR4712-66 \(1\)](#)
[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
EcoRI 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
EcoRI (a)	0.5 µL	0.5 µL	0.5 µL	-	-	-	0.5 µL	-	-	-	-
NcoI	-	-	-	0.5 µL	0.5 µL	0.5 µL	0.5 µL	-	-	-	0.5 µL
EcoRI (b)	-	-	-	-	-	-	-	0.5 µL	0.5 µL	0.5 µL	0.5 µL

EcoRI (a) assay date 2/05

EcoRI (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 \(Formatting\) \(1\)](#)
[Software discussions \(2\)](#)
[Starting materials and reagents \(1\)](#)

Lab Book Ref

[JR4712-63 \(1\)](#)
[JR4712-64 \(2\)](#)
[JR4712-66 \(1\)](#)
[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 \(1\)](#)

29 Jan 2007



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Mutagenesis of plasmid p042 via Taq and GenemorphI

9th January 2007 @ 14:34

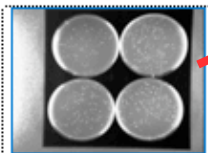
Lab Book Ref: jrh4712-78

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	-	-
MgCl ₂	2.5 µL	-	3.5 µL	3.5 µL
MnCl ₂	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.

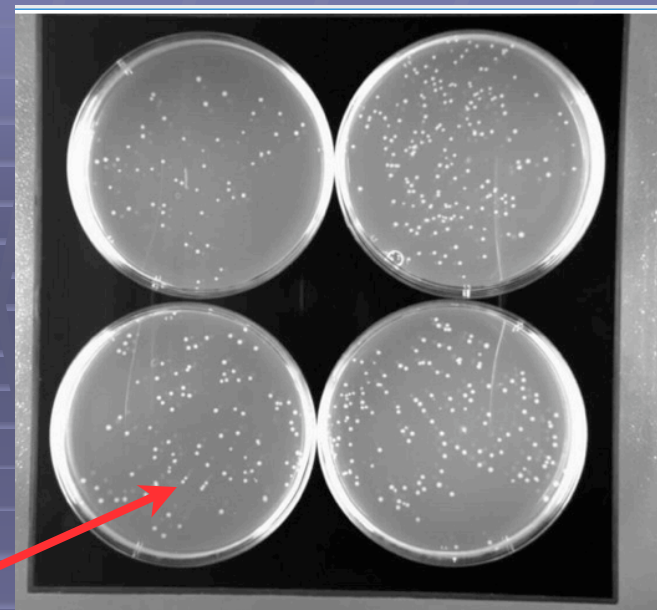
The reactions were run on program MUTAGGG for 30 cycles. 5 µL product was run on a 1% normal agarose analytical gel. Taq mutagenesis had failed, Genemorph and +ve ctrl had worked. -ve control was correct.



Jennifer Hale | [Beta-glucuronidase](#) | [Comments \(3\)](#)

[<< Previous Page](#)

[Next Page >>](#)



29 Jan 2007



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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 purify 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

Links

Admin

[New Post](#)

Live Copy



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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 available. 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

Links

‘Blog-jects’

29 Jan 2007



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University of Southampton

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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



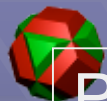
Blog-jects

- 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

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People



BLOG

Lab
Rep.

Instruments

E-print
Rep.

Broker

BLOG

Transformation
Agents

Sensors

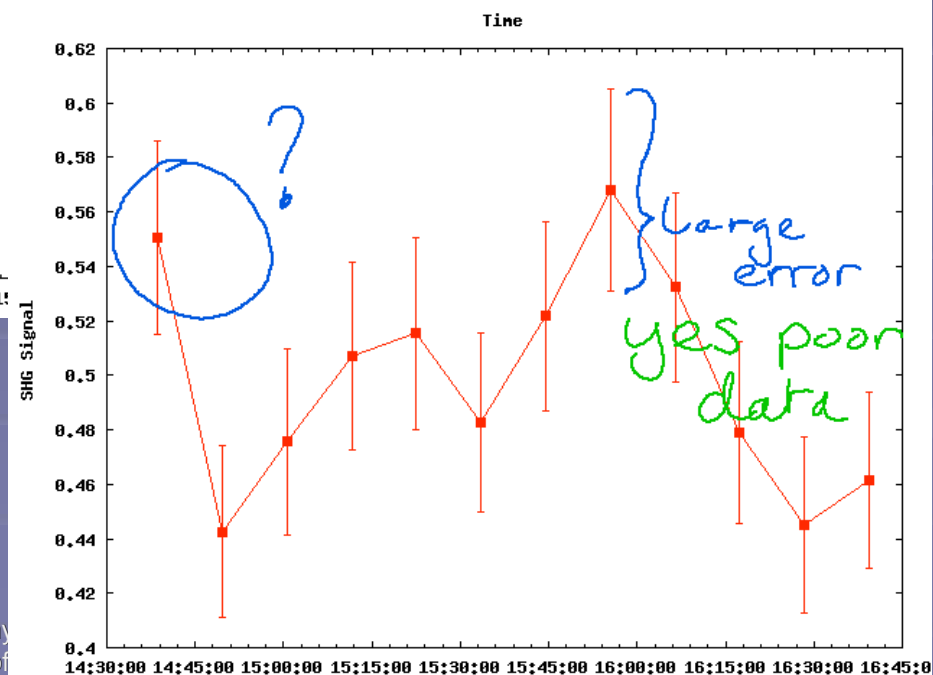
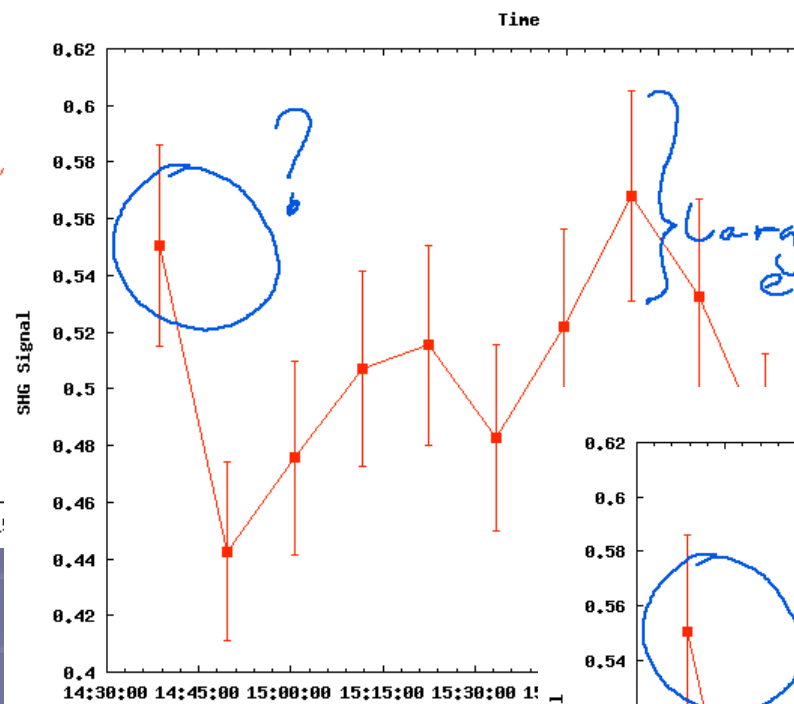
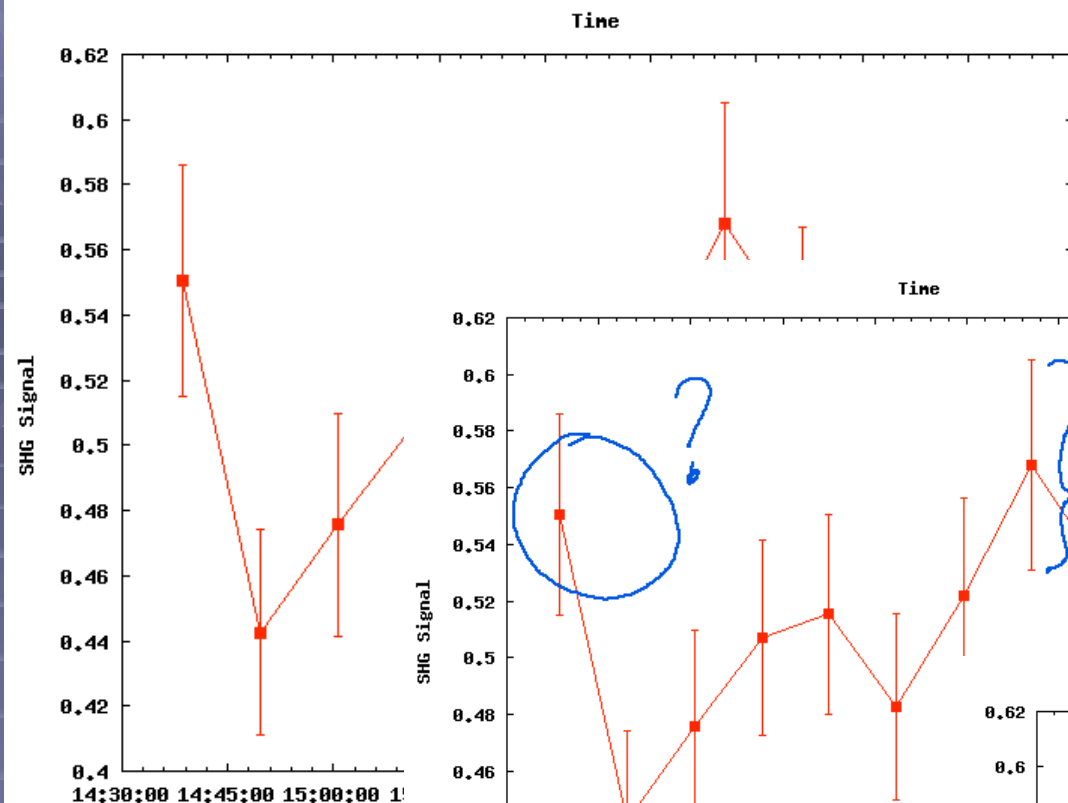
Archive

29 Jan 2007



Jeremy G. Frey
University of Southampton

Web 2.0 Workshop



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

29 Jan 2007



Jeremy
University of

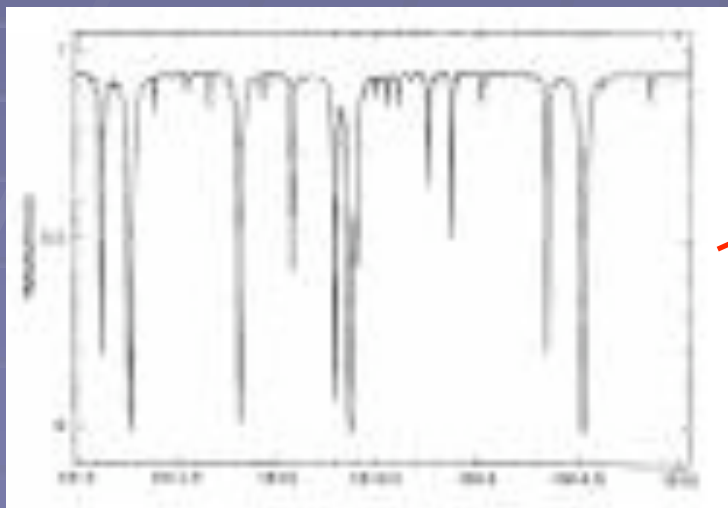
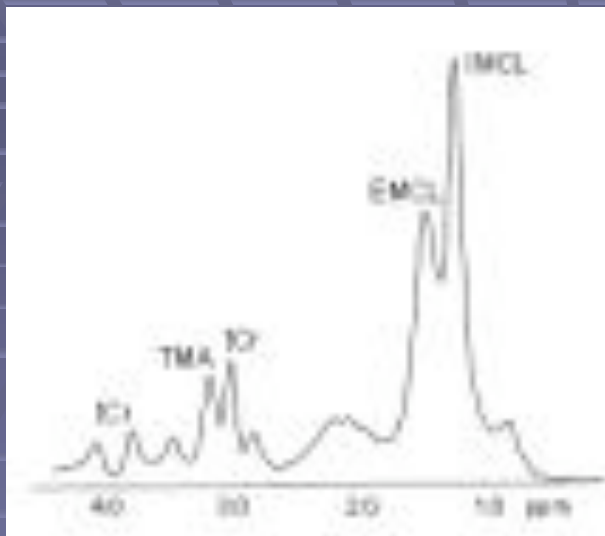


Validation

- 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



Why? Publishing Data and Information Loss



BY NC SA

b515548g.pdf (application/pdf Object) - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://www.rsc.org/efj/DT/2006/b515548g.pdf

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NCS Dalton Transactions Articles b515548g.pdf (application/pdf Objec...

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Search Web YAHOO! TOOLBAR Get it free

Pages

Comments

Attachments

by passing through columns of P_2O_5 with moisture indicator and 4 Å molecular sieves and permeation chromatography (GPC) measurements were performed on a Polymer Laboratories PL-GPC-220 instrument equipped with a PL-gel 5 Å Mixed-C column, a refractive index detector, and a PD2040 light scattering detector. The GPC column was calibrated using eight monodisperse polystyrene standards in the range 580–48300 Da.

Preparation of $CPh_3[NCPBB]$ (1)

Potassium cyanide (33.6 mg, 0.5 mmol) was ground to a powder using a pestle and mortar in a dry box. PBB (0.478 g, 0.5 mmol) and 50 mL diethyl ether were then added, and the mixture was heated to reflux for 12 h. The solvent was removed *in vacuo* to leave an off-white foam which was washed with warm hexane (50 mL) to give $K[NCPBB]$ as a white powder (0.495 g, 485 μmol). This solid was stirred with triphenylchloromethane (0.135 g, 0.485 mmol) in dichloromethane (15 mL) for 2 h. The solution was filtered to remove KCl, concentrated to ca. 5 mL and cooled to $-26^\circ C$ to give an orange crystalline solid, yield: 0.324 g (0.315 mmol, 63% with respect to KCN). IR (nujol): 2189 cm^{-1} (ν_{CN}). 1H NMR (CD_2Cl_2 , $20^\circ C$, 300.13 MHz): δ 8.28 (t, 3 H, $J = 7.5$ Hz, *p*-Ph), 7.90 (t, 6 H, $J = 7.5$ Hz, *m*-Ph), 7.70 (d, 6 H, $J = 7.3$ Hz, *o*-Ph). ^{13}C NMR (CD_2Cl_2 , $20^\circ C$, 75.48 MHz): δ 211.4 (CPh_3), 144.0 (*p*-C), 143.0 (*m*-C), 140.3 (*ipso*-C), 131.0 (*o*-C), 153.6, 150.3, 147.5, 146.4, 140.3, 139.6, 136.9, 136.3, 128.3, 113.5, 109.5 (Ar C-F). ^{19}F NMR (CD_2Cl_2 , $20^\circ C$, 96.3 MHz): δ -16.2 (br s).

Preparation of $CPh_3[(C_6F_5)_2BCNPBB]$ (2)

$Me_3SiNCB(C_6F_5)_2$ (0.51 g, 0.84 mmol) and Ph_3CCl (0.23 g, 0.84 mmol) were stirred in 20 mL of dichloromethane for 0.5 h to give a yellow solution. After removal of volatiles *in vacuo*, the residue was washed with pentane (30 mL), PBB (0.81 g, 0.84 mmol) and dichloromethane (30 mL) were added, and the mixture was stirred for 2 h. The solvent was then removed. The product was washed again with 30 mL of pentane and dried *in vacuo* to yield a yellow-orange powder (yield 1.01 g, 5.8 mmol, 69%). Attempts to recrystallise the product from dichloromethane were not successful. IR (nujol): 2284 cm^{-1} (ν_{CN}). 1H NMR (CD_2Cl_2 , $20^\circ C$, 300.13 MHz): δ 8.56 (t, 3, $J = 8.0$ Hz *p*-Ph), 7.90 (t, 6 H, $J = 7.5$ Hz, *m*-Ph), 7.70 (d, 6 H, $J = 7.2$ Hz, *o*-Ph). ^{13}C NMR (CD_2Cl_2 , $20^\circ C$, 75.48 MHz): δ 211.0 (CPh_3), 144.1 (*p*-C), 143.0 (*m*-C), 140.1 (*ipso*-C), 130.9 (*o*-C). ^{19}F NMR (CD_2Cl_2 , $20^\circ C$, 96.3 MHz): δ -4.35 (s, br, 1 B, N- $B(C_6F_5)_2$), -18.27 (s, 1 B, $C-B(C_6F_5)_2$). ^{19}F NMR (CD_2Cl_2 , $20^\circ C$, 282.4 MHz): δ -118.72 (br, s, 1 F), -120.22 (br, s, 1 F), -121.99 (br, s, 1 F), -122.50 (s, 1 F), -132.20 (s, 1 F), -133.94 (br, 6 F, *o*-F on $B(C_6F_5)_2$), overlapping signals (-134.15, -134.39, -134.95, -135.27, -135.64), 136.89 (br, 1 F), -137.81 (br, 3 F), -138.79 (d, 1 F), -144.73 (t, 1 F), -149.78 (t, 1 F), -151.11 (t, 1 F), -154.65 (t, 1 F), -154.93 (t, 1 F), -155.32 (t, 1 F), -156.86 (t, 1 F), -157.24 (t, 1 F), -157.55 (t, 1 F), -158.29 (m, 1 F), -158.90 (t, 1 F), -159.57 (t, 3 F, $J = 20$ Hz, *p*-F on $B(C_6F_5)_2$), -159.98 (t, 1 F), -161.44 (br, 2 F), -164.0 to -164.4 (overlapping signals, 3 F), -165.33 (br, 2 F), -166.12 (t, 3 F, $J = 20$ Hz, *m*-F on $B(C_6F_5)_2$). Anal. Calcd for $C_{24}H_{15}B_2F_{12}N$:

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9 of 12

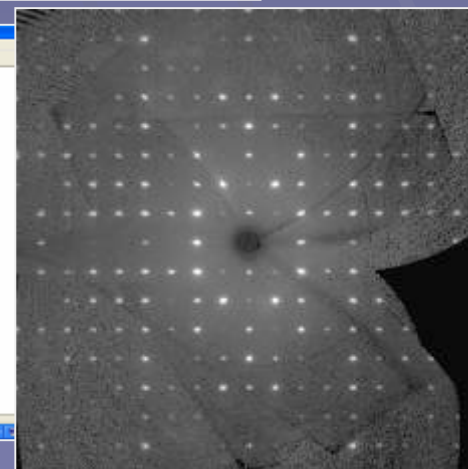
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Jeremy G. Frey
University of Southampton

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Access to **ALL** underlying data

Southampton Crystal Reports - Benzene 1,7dicarboxylic acid - Microsoft Internet Explorer

Address: <http://crystals.chem.soton.ac.uk/149/>

Chemical formula	C8 H6 O4
Crystallisation Solvent	
Crystal morphology	Prism
Crystal system	monoclinic
Space group symbol	C2/c
Cell length a	5.0016(10)
Cell length b	14.214(3)
Cell length c	9.5196(19)
Cell angle alpha	90.00
Cell angle beta	94.33(3)
Cell angle gamma	90.00
Data collection temperature	120(2)
Refinement results	
Solution figure of merit	0.0354
R Factor (Obs)	0.0423
R Factor (All)	0.0534
Weighted R Factor (Obs)	0.1116
Weighted R Factor (All)	0.1197

Available Files

Final Result

- 05mbh1006.cml 3k
- 05mbh1006/05mbh1006.cif 9k
- 05mbh1006/05mbh1006_checkcif.htm 7k
- 05mbh1006_inchi.cml 1k

Refinement

- 05mbh1006/05mbh1006.res 3k
- 05mbh1006/05mbh1006_xl.lst 21k

Solution

- 05mbh1006/05mbh1006.prp 5k
- 05mbh1006/05mbh1006_xs.lst 30k

Processing

- 05mbh1006/05mbh1006.hkl 106k
- 05mbh1006/05mbh1006.htm 10k
- 05mbh1006/05mbh1006_0kl.jpg 67k
- 05mbh1006/05mbh1006_h0l.jpg 84k
- 05mbh1006/05mbh1006_hk0.jpg 63k

Data Collection

- 05mbh1006/05mbh1006_crystal.jpg 1k

Other Files

- 05mbh1006/05mbh1006.doc 63k
- 05mbh1006/05mbh1006.rcf 39k
- 05mbh1006/05mbh1006.ins 2k
- 05mbh1006/05mbh1006.mol 1k
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Summary report for Directory: diska/02sot082

Report generated Jul 09, 2002, 10:13:51

Unit cell

15124 reflections with 2.91°-delta=27.48° (resolution between 7.00Å and 0.77Å) were used for unit cell refinement

Symmetry used p222

in scalepack

a (Angstrom) 9.3133 +/- 0.0003

b (Angstrom) 9.8424 +/- 0.0003

c (Angstrom) 15.4441 +/- 0.0004

alpha (°) 90.000

beta (°) 90.000

gamma (°) 90.000

Volume (Å³) 1415.69 +/- 0.07

Mosiacity (°) 0.743 +/- 0.002

EPSRC National Crystallography Service

Data Collection Summary

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Report generated Jul 09, 2002, 10:13:51

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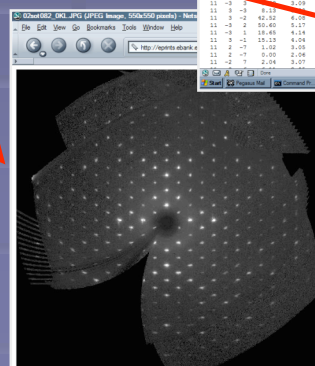
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gamma (°) 90.000

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29 Jan 2007

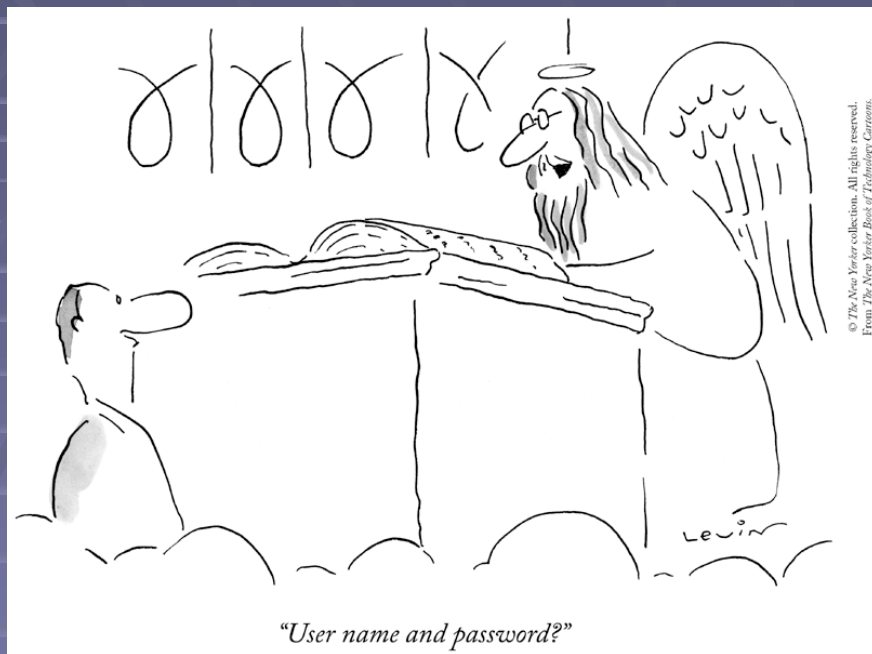


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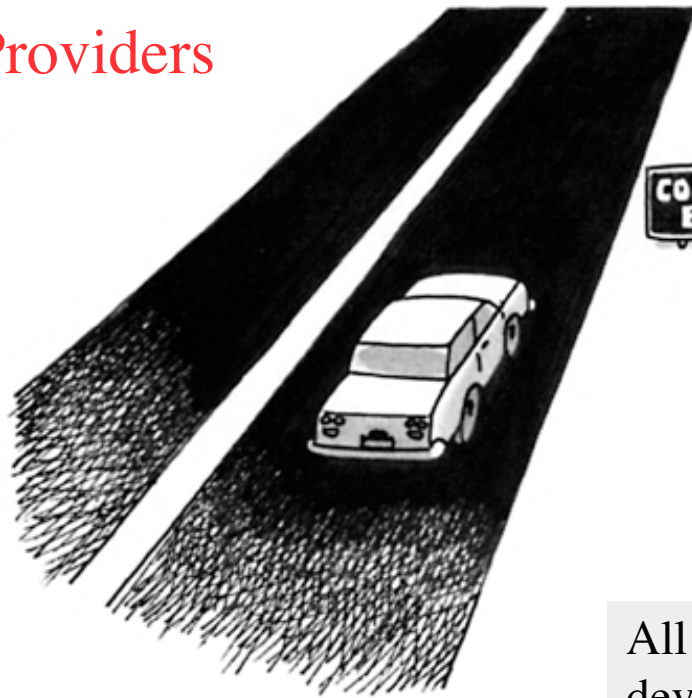
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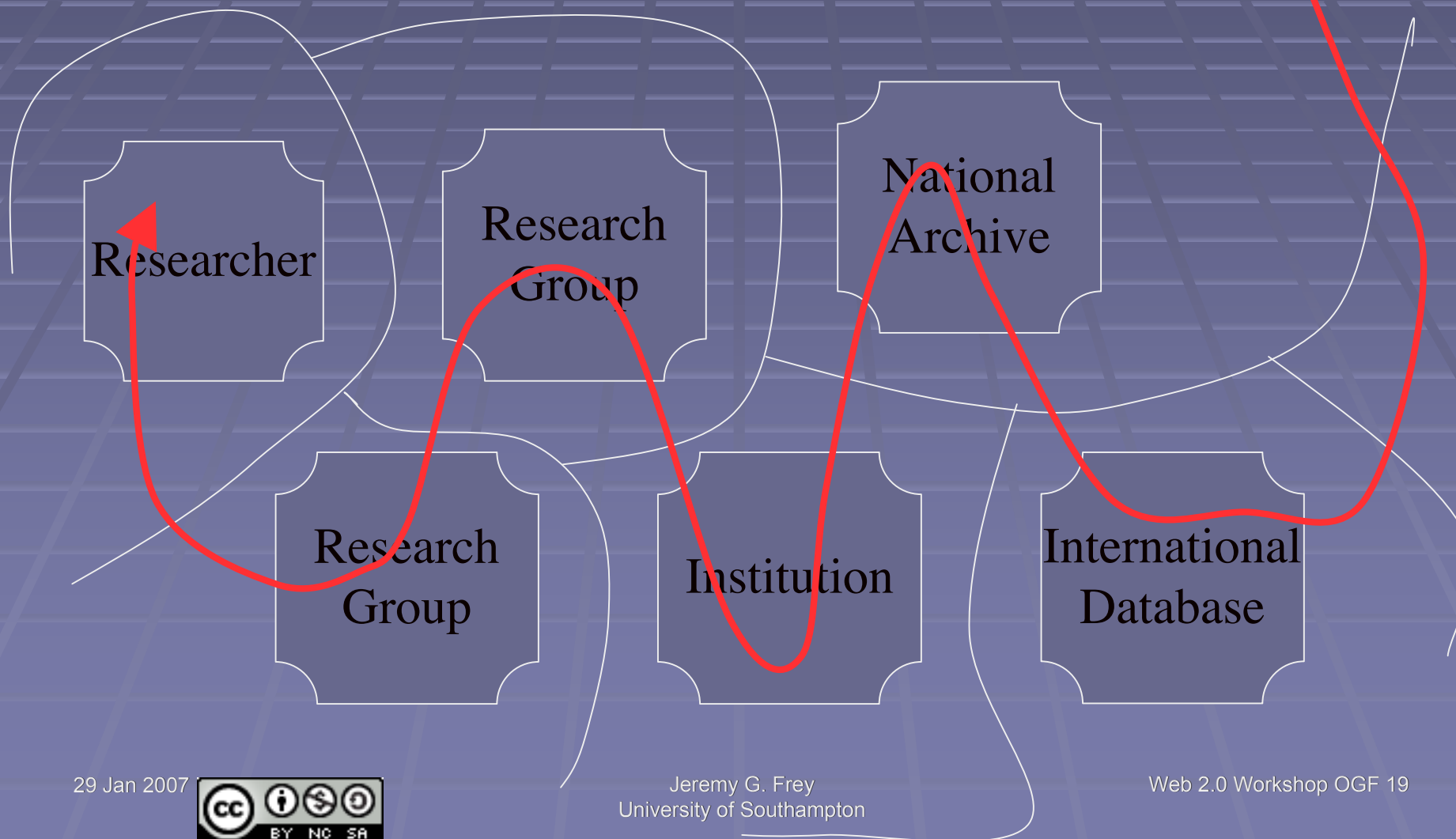


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All I am saying is that now is the time to
develop the technology to deflect an asteroid



Access to information requires crossing administrative domains





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