

Future Lab - "Smart Not Dark"

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16 Feb 2006
Smart Lab

Laboratory Informatics Exchange 2006



The CombeChem Project

- 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
- End to End linking of data and information
 - Publication@Source
- But then.... "Who needs provenance?"
Bush, Blair The JIC, MI5, CIA & Hutton



Chemical Grids

- Start in the laboratory – pervasive physical grid (Smart Tea)
- Computational chemistry very significant source – *in silico* grid (Chem MyTea)
- Used by chemists so must be simple to support & maintain - *simple, stable, secure, & autonomic*

What are the people up to?

We can capture the environment
but need to capture the processes

Who is doing what, where are
they doing it, and what is the
environment like?

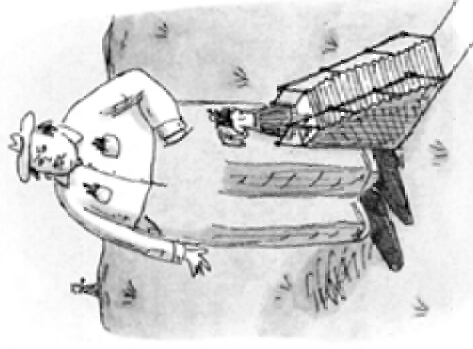


Like cash machine
electronic notebooks
have taken many forms
- we want one that
adapts to context,
simple to use in the lab
whilst doing actual
bench chemistry but
linked to more
resources at the desk -
the pervasive lab book
grid

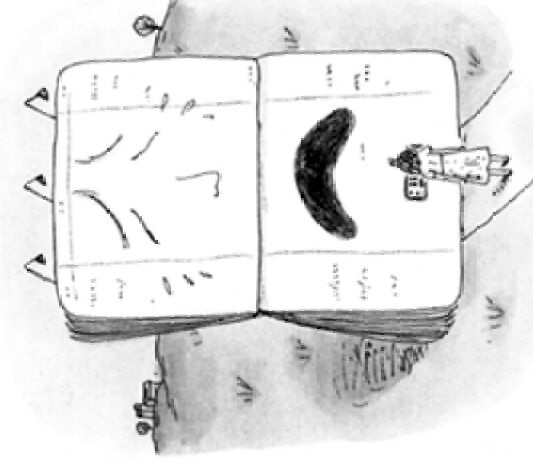
CASH MACHINES ~~from~~ ACROSS THE LAND



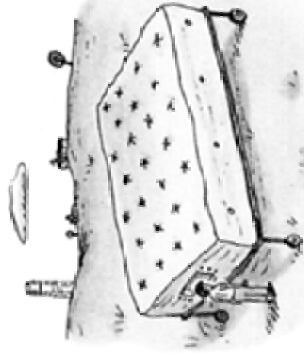
The Big Purse
East Lubbock, New Jersey



Dad's Pocket Cashometer
Twelve Buckets, Nebraska



The Weeping Bankbook
Henrieville, Alabama



Mattress o' Moola
Knool, Idaho

R. G. Root

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From The New Yorker Book of Technology Cartoons

ChemLab

The Chemistry 3/5 & 6
Laboratories

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

DARTMOUTH COLLEGE

Safety

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

Resources

[Applets](#)
[General FAQ](#)
[Uncertainty](#)

[ChemLab Home](#)

Permanent,
documented
and primary
record of
laboratory
observations

16 Feb 2006

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.



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.

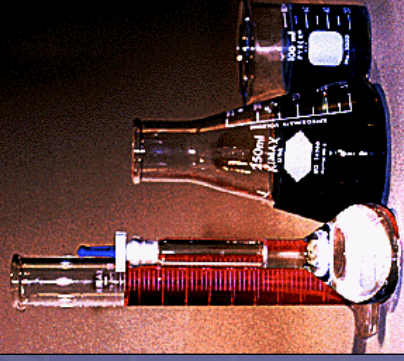
Each week at the beginning of lab lecture, you will turn in your prelab problems from the manual for grading. Problems not turned in at the beginning of lab lecture will be

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

ChemLab

The Chemistry 3/5 & 6
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- ▶ Chemistry 6 Experiments



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University of Southampton

Mathematics
Exchange

Industrial supporte



critical data
entry



COSHH

leverage off things we already have to do

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





Weigh-Station #1

11-Feb-2004 16:04:40

dj

djbj3403

Experiment Details

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	40.0 ml

7	8	9
4	5	6
1	2	3
0		.

Enter	Del
-------	-----

All measurements completed.

djbj3	Merck2	Potassium Carbonate	Butanone
-------	--------	---------------------	----------

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Quit

Weigh

Liquid-Measure

Bench

Store

Escape



Ingredient List

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

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	40.0 ml

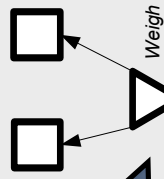
Dissolve 4-fluorinated biphenyl in butanone

Add K₂CO₃ powder

Heat at reflux for 1.5 hours



0.9031 grammes

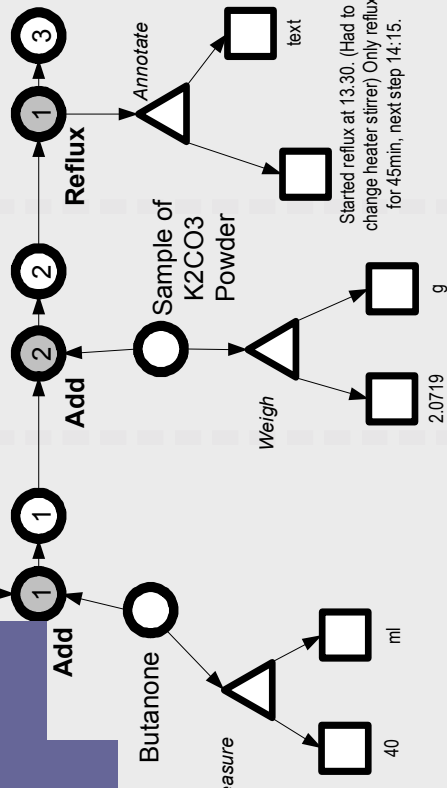


Sample of 4-fluorinated biphenyl

7	8	9
4	5	6
1	2	3
0	.	

Enter

Del





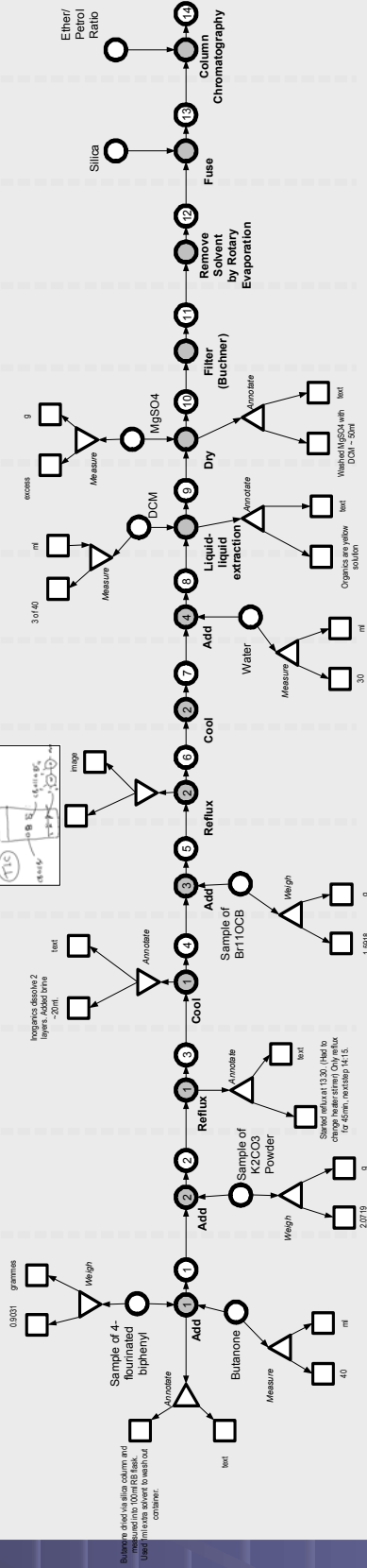
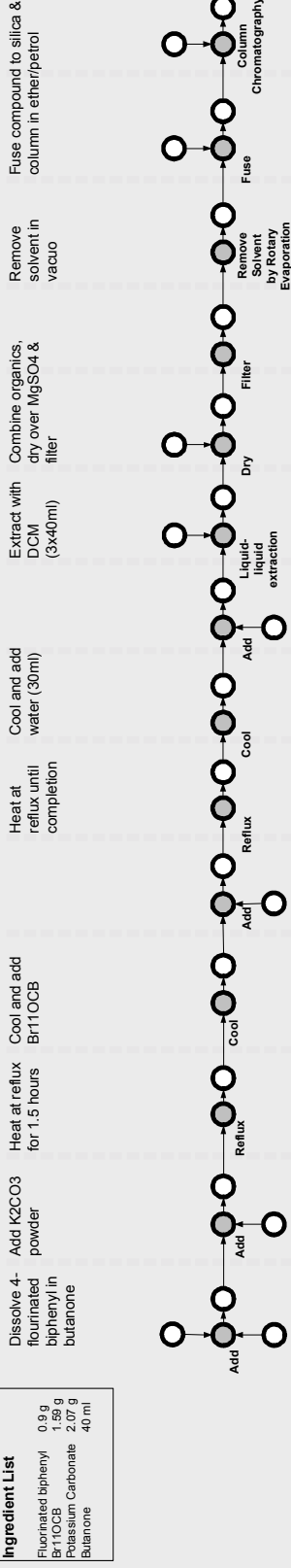
To Do

Plan

Process Record

Ingredient List

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



Key

- Process
- Input
- Literal
- Observation

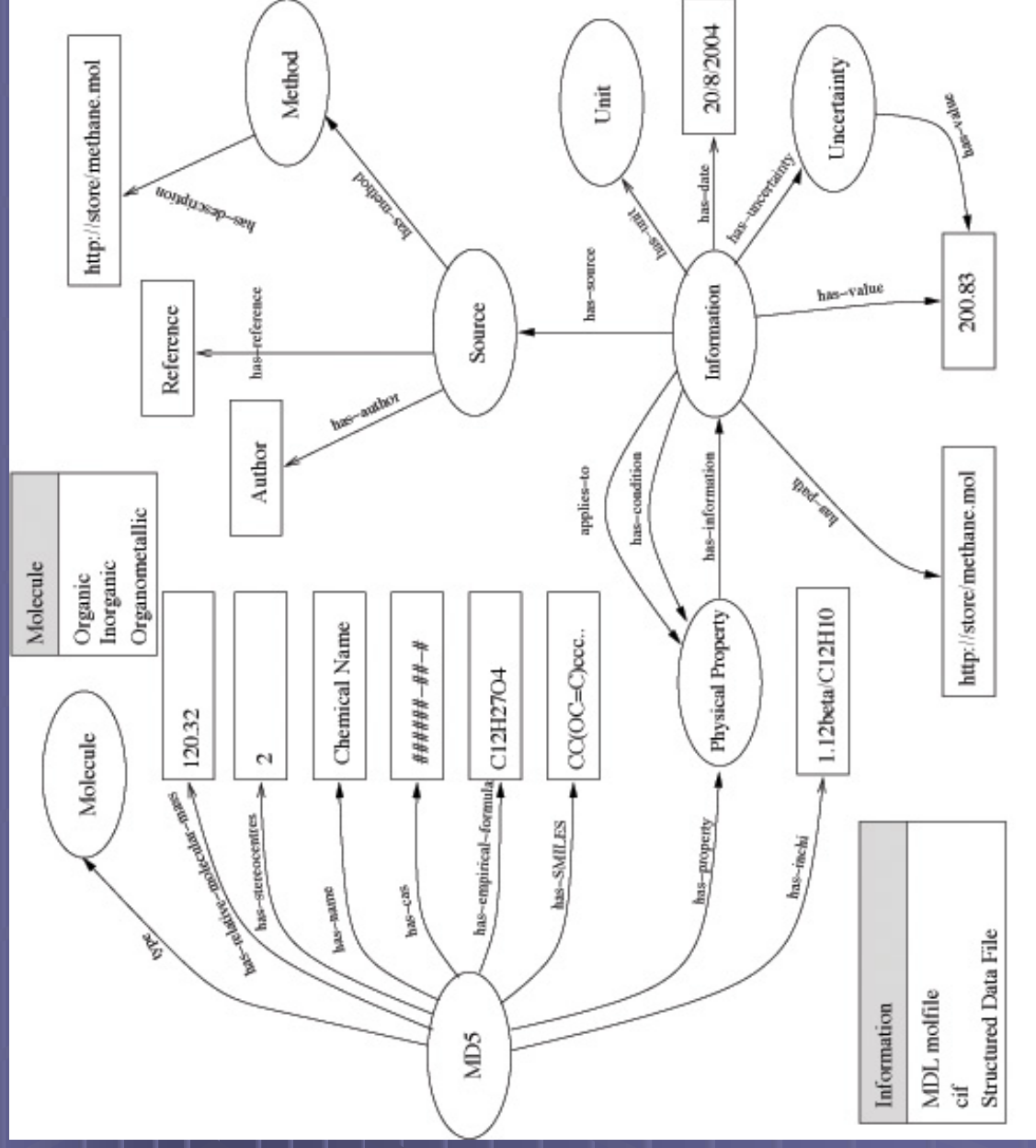
Observation Types

- 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
gyh, hrm, gms





Property in RDF

- `<c:OrganicMolecule rdf:about="file:///storage/ba8efc2ce0edada69d63b02d1b8630c6.rdf">`
- `<c:has-inchi>I.12Beta/C12H13NO2/c1-2-15-8-9-5-6-11(14)12-10(9)4-3-7-13-12/h1H3,2H2,3-7H,8H2,14H</c:has-inchi>`
- `<c:has-cas>22049-19-0</c:has-cas>`
- `<c:has-empirical-formula>C12H13NO2</c:has-empirical-formula>`
- `<c:has-stereocentres>0</c:has-stereocentres>`
- `<c:has-property>`
- `<c:MeltingPoint>`
- `<c:has-information>`
- `<c:Information>`
- `<c:has-value>150</c:has-value>`
- `<c:has-uncertainty>`
- `<c:Range>`
- `<c:has-value>16</c:has-value>`
- `</c:Range>`
- `<c:has-uncertainty>`
- `</c:Information>`
- `</c:has-information>`
- `</c:MeltingPoint>`
- `</c:has-property>`
- `</c:OrganicMolecule>`



Schema

- `<rdfs:Class rdf:about="&c;OrganicMolecule">`
- `<rdfs:label>Organic Molecule</rdfs:label>`
- `<rdfs:subClassOf rdf:resource="&c;Molecule" />`
- `</rdfs:Class>`
- `<rdfs:Class rdf:about="&c;PhysicalProperty">`
- `<rdfs:label>Property</rdfs:label>`
- `</rdfs:Class>`
- `<rdfs:Class rdf:about="&c;PartitionCoefficient">`
- `<rdfs:label>Partition Coefficient</rdfs:label>`
- `<rdfs:subClassOf rdf:resource="&c;PhysicalProperty" />`
- `<rdfs:description>Ratio of substance dissolved in octan-1-ol and water</rdfs:description>`
- `</rdfs:Class>`

This turns out to be a very flexible approach

File Edit View Go Bookmarks Tools Window Help

file:///rob/prog/triangle/test2/nitrostyrene-page.htm

Search

1202-32-0

CAS INCHI NAME SMILES CEMPIR

Search the DB

Canned Example

query number = [10]

• MOLECULE

type	Resource
type	Molecule
has-SMILES	<chem>c1ccccc1C=C(C(=O)N)=O</chem>
has-name	B-ETHYL-B-NITROSTYRENE
has-mmm	177.2
has-stereocentres	0
has-empirical-formula	C10H11NO2
has-cas	1202-32-0

has-property

48.29587

type PhysicalProperty

type BoilingPoint

type Resource

has-information

49.29587

type Resource

type Information

has-date 2003-2-28

has-value 307.3

has-uncertainty

has-unit

has-source

53.29587

type Source

type PhysProp

type Resource

has-method

54.29587

type Resource

type Laboratory

of-quality

has-condition

has-property

16.29587

type PhysicalProperty

type Solubility

type Resource

file:///rob/prog/triangle/test2/nitrostyrene-page.htm

Search

nitrostyrene

has-property

28.26097

type BoilingPoint

type PhysProp

type Resource

has-information

8.26587

type BoilingPoint

type PhysProp

type Resource

has-information

Chemical structure of nitrostyrene (B-ethyl-b-nitrostyrene) is shown.

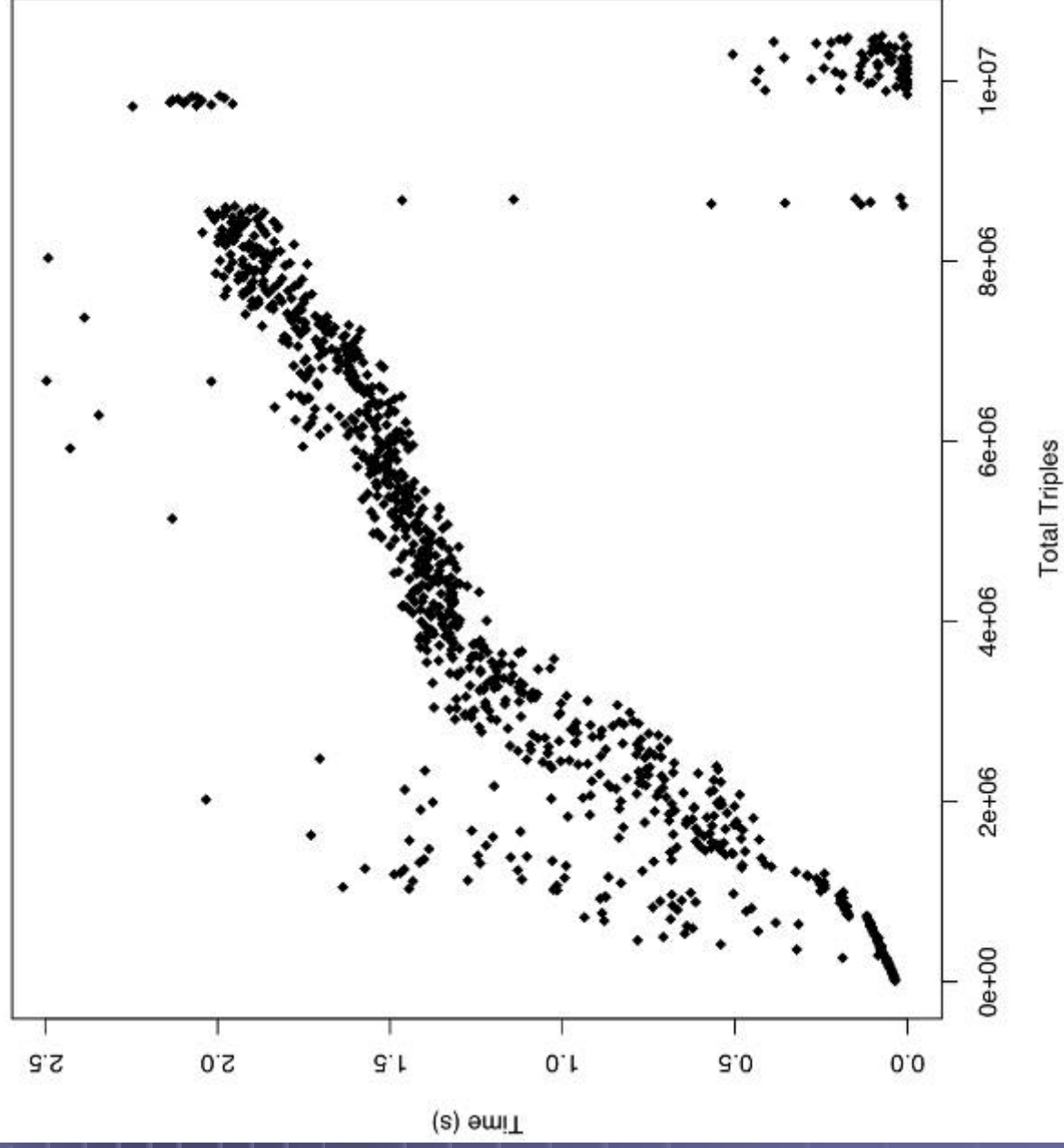
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ACCESS RESTRICTED
Version 1.0.6

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Performance of Six Related Queries





Adapt SHG lab

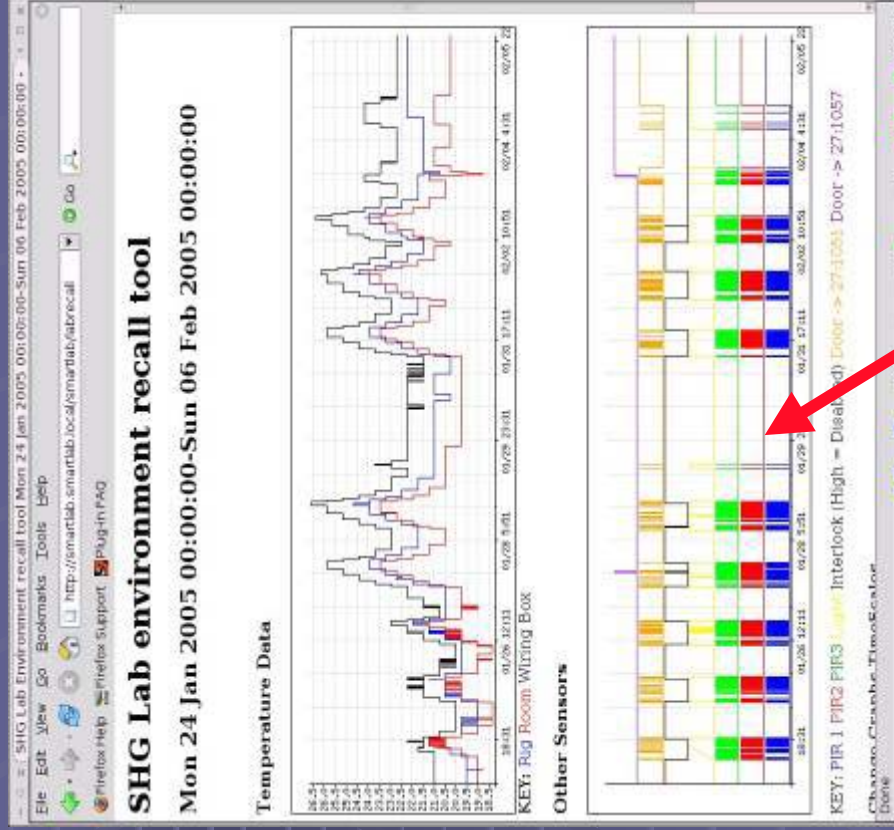
- Capture information from places you would not want to put your eyes



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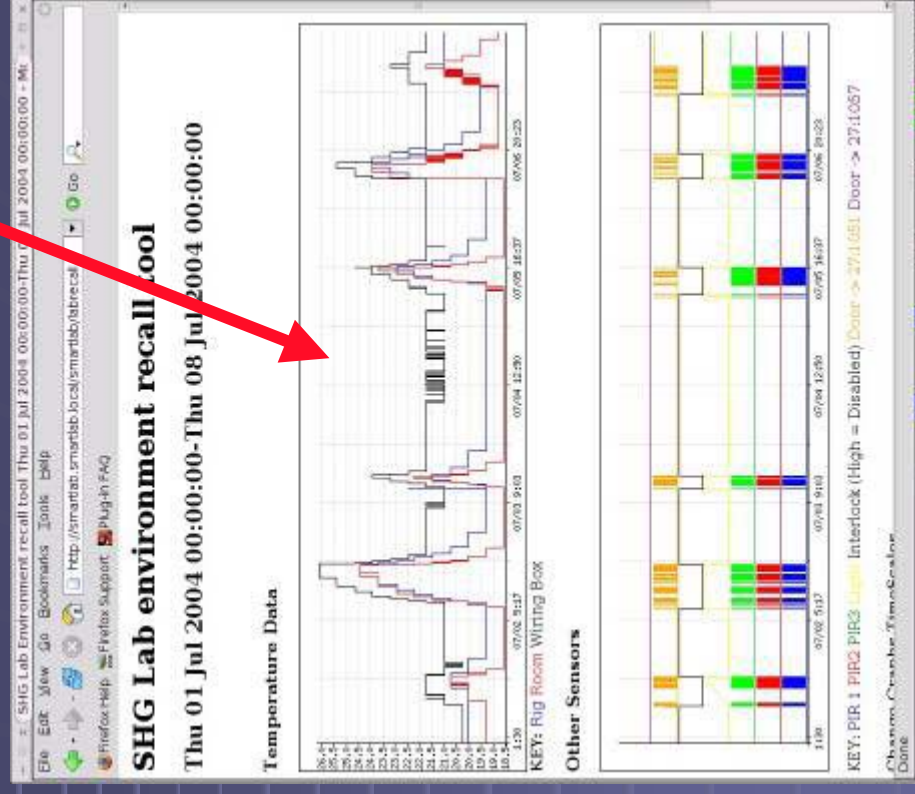
Air Conditioning failed

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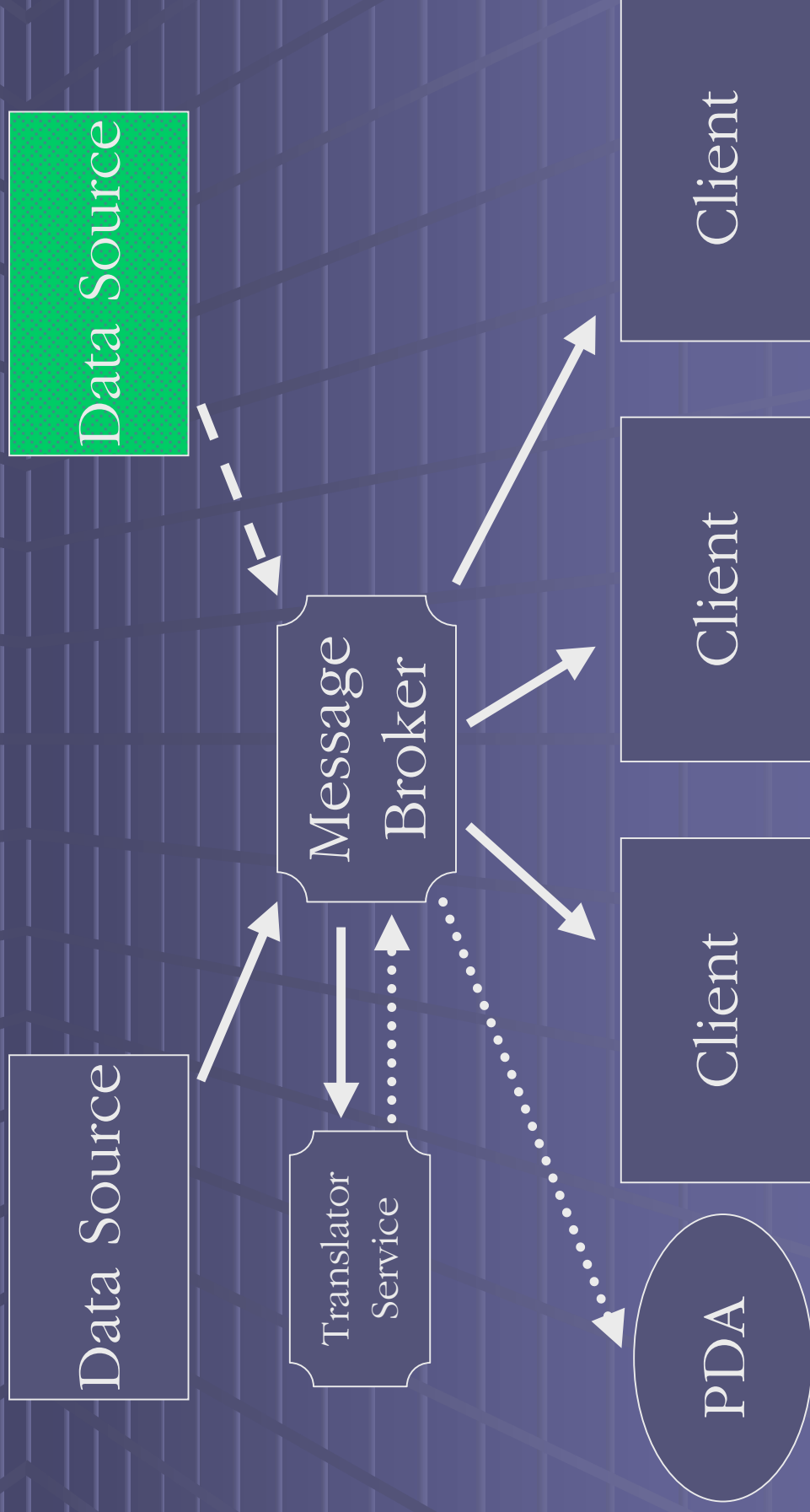
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Student turned off a/c





Get the view of the lab where and when you want
in the way you want it - how to support this





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Last Updated: Fri 11 Feb 2006 11:05 AM

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Chemists

By Jo Twist
BBC News science editor

A blend of mobile technology and award-winning science is letting scientists escape the lab

The software, "middleware", other secure computer systems and instantaneous data transfer are the key to the project.

As part of a project in the UK, scientists are using mobile phones to let scientists escape the lab.

Sensors in the mobile phones can detect changes in the lab environment and the system can alert scientists.

"It replaces the need for a dedicated mobile phone system."

PDAs everywhere

Members of Dr Frey's non-linear laser spectroscopy research group, working as part of the Combechem project, have been successfully trying out the system at conferences - and in the university bar.

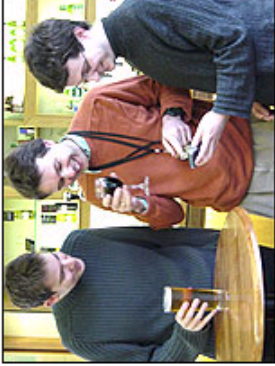
The next step is to evolve the system so that at a push of a button on a mobile, scientists will be able to remotely change the conditions in the lab, like turning down the temperature.

It could also realise the promise of controlling home environments from phones easily and seamlessly.

But there are many other potential applications for the monitoring jobs done by the power industries, healthcare professions and other labs.

IBM won the Royal Academy of Engineering's MacRobert prize which rewards technological and engineering innovation for the program in June last year.

Used by top global banks, the WebSphere MQ family is a decade old.



Chemists enjoy a drink at the bar while keeping an eye on the lab.

Address http://news.bbc.co.uk/1/hi/sci/tech/4233757.stm

http://news.bbc.co.uk/1/hi/sci/tech/4233757.stm

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