ELNs In the Semantic Era

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15 March 2006
IBC Life Sciences
Maximising the Potential of Electronic Laboratory Notebooks

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

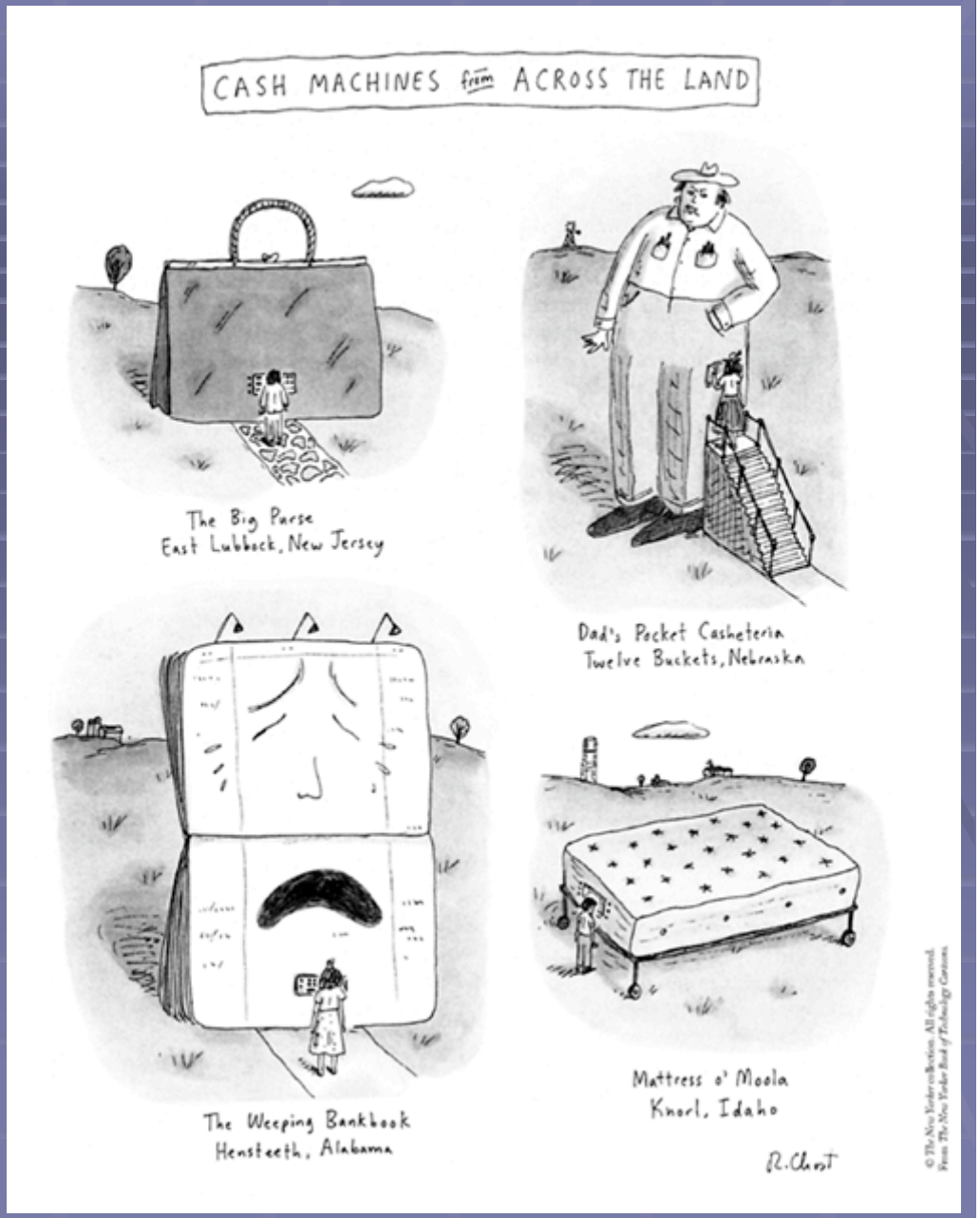
- Start in the laboratory – pervasive physical grid (Smart Tea)
- Computational chemistry very significant source – *in silico* grid (*Chem* MyTea)
- Used by chemists so must be simple to support & maintain - *simple, stable, secure, & autonomic*

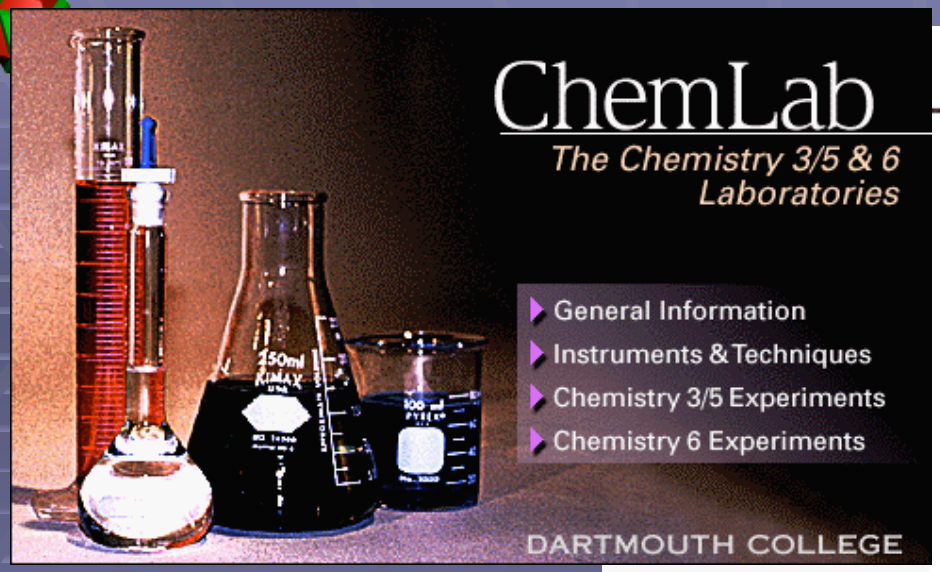
What are the people up to?

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





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

15 March 2006

Safety
General Rules
Safety Equipment
Safety Hazards
Procedures

Resources
Applets
General FAQ
Uncertainty

ChemLab Home

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.

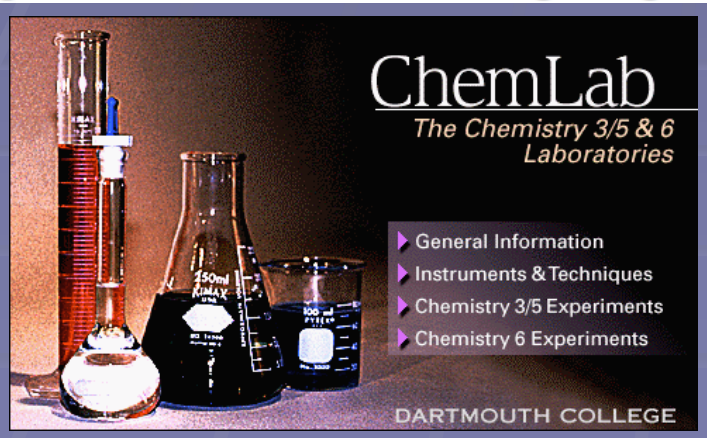
The laboratory notebook is a permanent, documented, and primary record of laboratory observations. Therefore, your notebook will be a bound journal with pages that should be numbered in advance and never torn out. A notebook will be supplied to you before the first laboratory period. Write your name, 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. [illegible] problems not turned in at the beginning of lab lecture [illegible] be

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



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Industrial support
GlaxoWellcome
critical data
entry

COSHH

leverage off things we already have to do

COSHH ASSESSMENT FORM Record No.

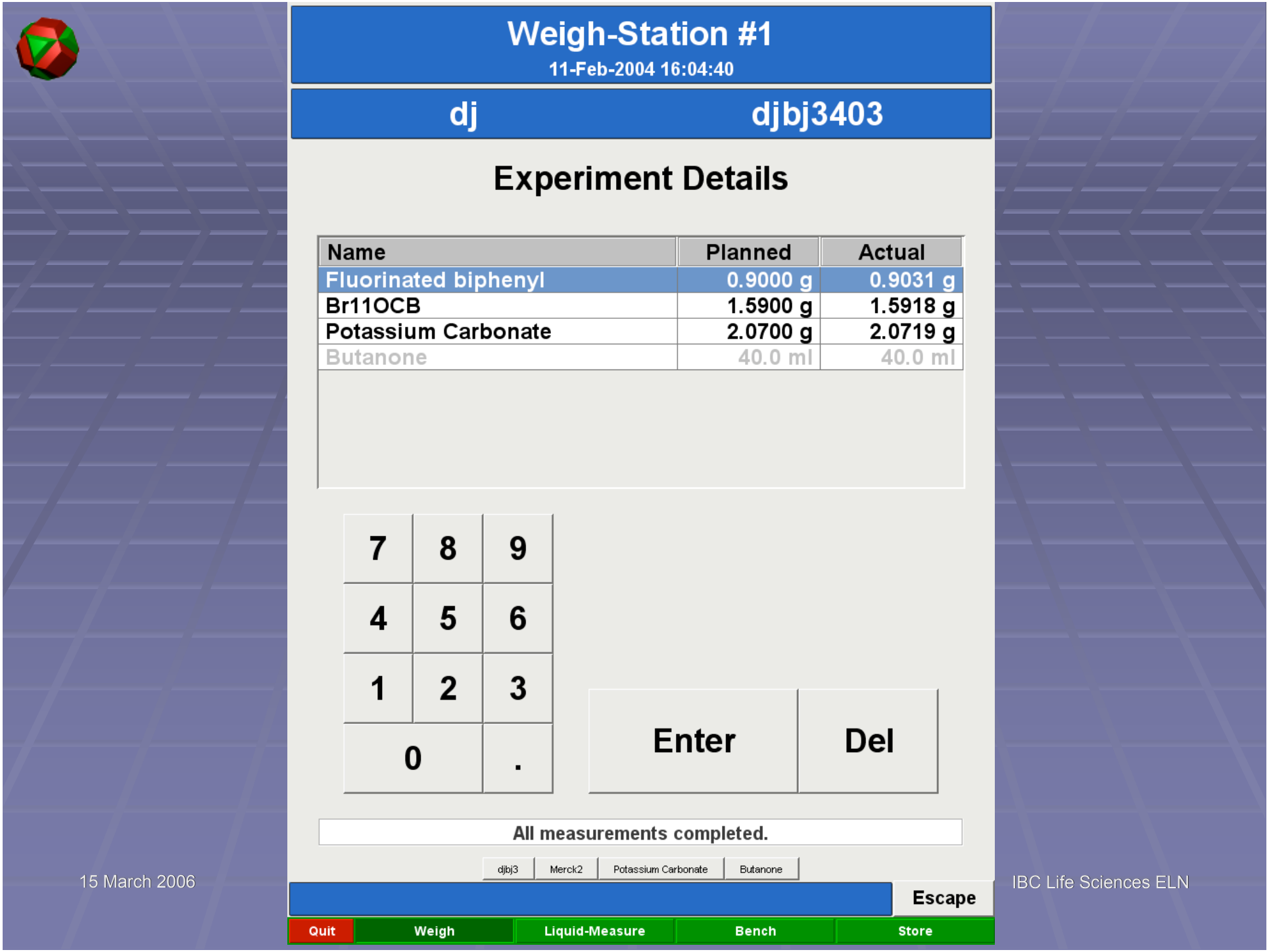
SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD
Water	liquid	1000ml	None
Dextrose	Solid	<20g	possible irritation to eyes and skin
Caffeine	Solid (tea)	<1g	Harmful if swallowed, induce vomiting
Milk	liquid	<100ml	No particular hazards

NATURE OF PROCESS

liquid extraction of caffeine, followed by combination with dext
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
Escape
Quit
Weigh
Liquid-Measure
Bench
Store

Ingredient List

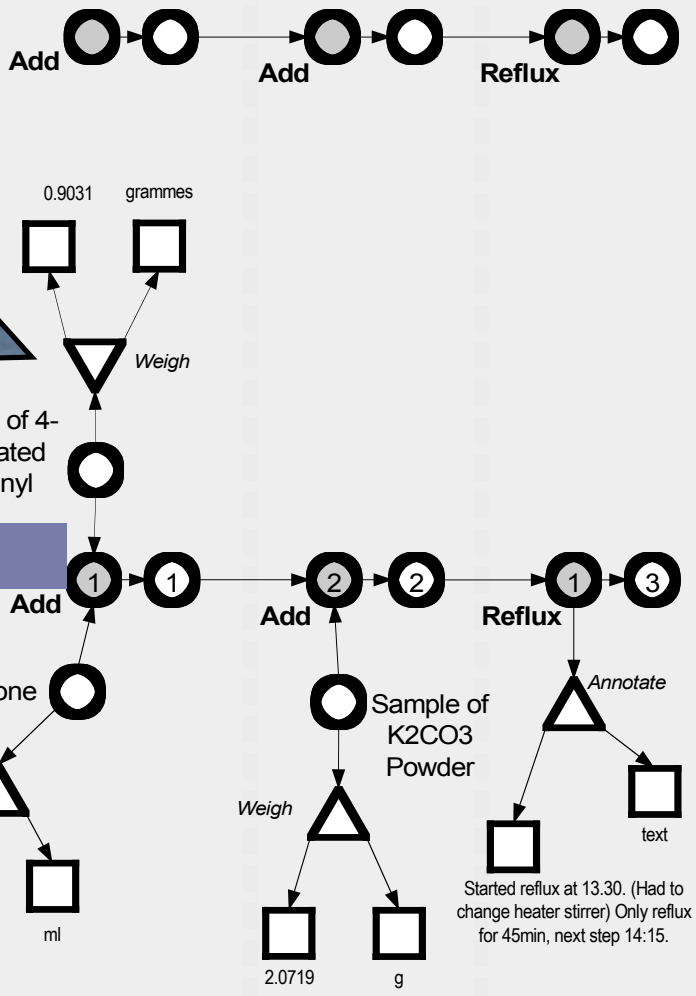
Fluorinated biphenyl	0.9 g
Br11OCB	1.59 g
Potassium Carbonate	2.07 g
Butanone	40 ml

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	40.0 ml



7	8	9
4	5	6
1	2	3
0		.

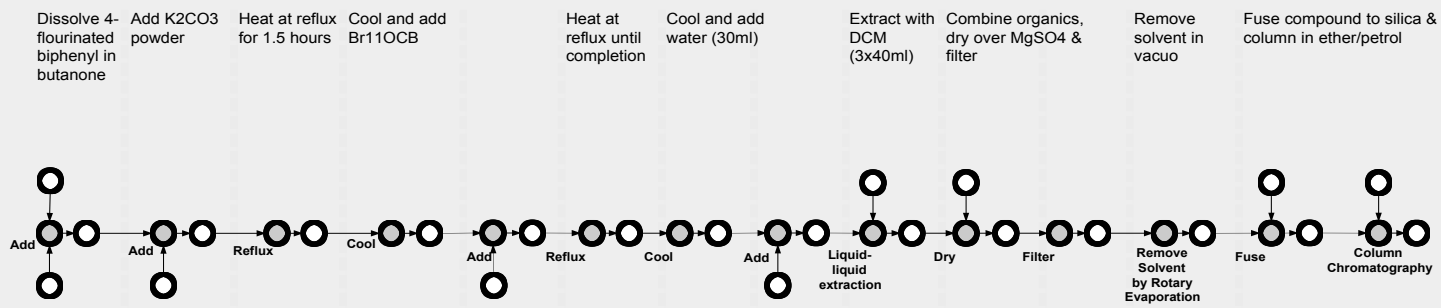
Enter | Del

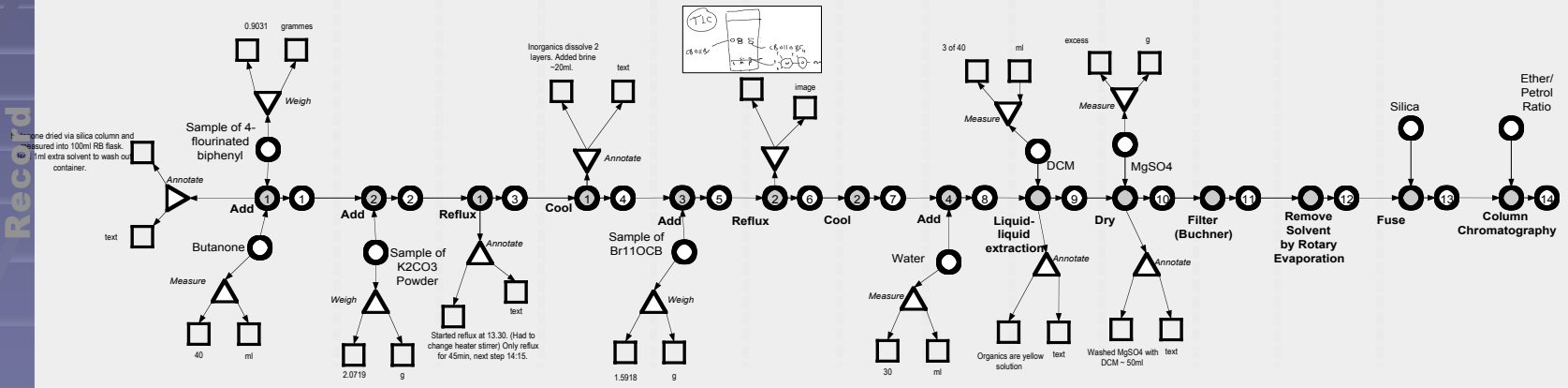
15 March 2006

To D
Lis
Plan
Process
Record

Ingredient List

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

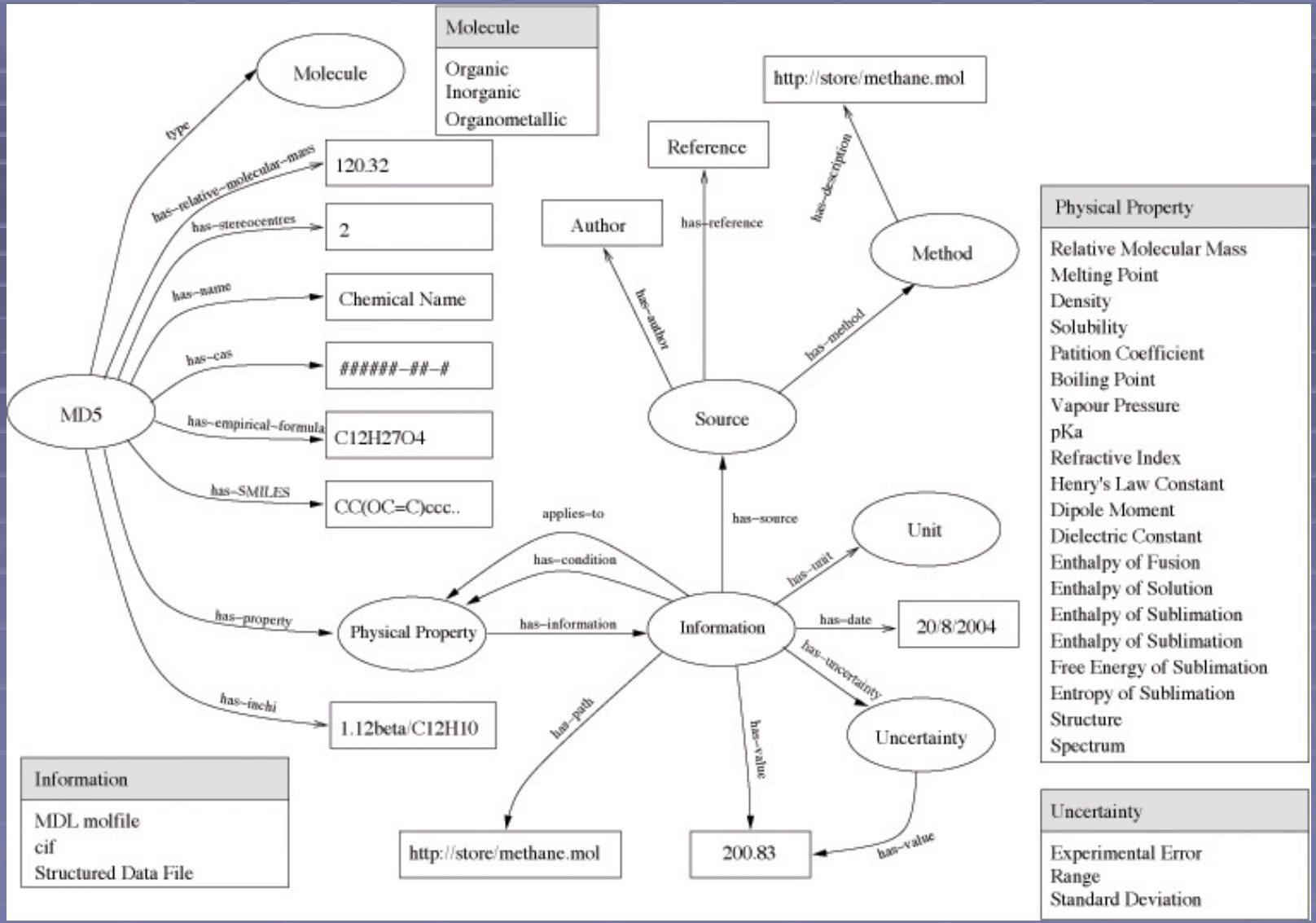
How to depict destructive processes

How to depict taking lots of samples

What is the observation/process boundary? e.g. MRI scan

Combechem

30 January 2004
gvh, hrm, gms


Molecule
Organic
Inorganic
Organometallic
Molecule
type
has-relative-molecular-mass
120.32
has-stereocentres
2
has-name
Chemical Name
has-cas
######-##-#
has-empirical-formula
C12H27O4
has-SMILES
CC(OC=C)ccc..
MD5
has-property
has-inchi
1.12beta/C12H10
Physical Property
has-information
Information
applies-to
has-condition
has-source
Source
Author
has-author
Reference
has-reference
http://store/methane.mol
has-description
Method
has-method
Unit
has-unit
has-date
20/8/2004
has-uncertainty
Uncertainty
has-value
200.83
has-path
http://store/methane.mol
Physical Property
Relative Molecular Mass
Melting Point
Density
Solubility
Patition Coefficient
Boiling Point
Vapour Pressure
pKa
Refractive Index
Henry's Law Constant
Dipole Moment
Dielectric Constant
Enthalpy of Fusion
Enthalpy of Solution
Enthalpy of Sublimation
Enthalpy of Sublimation
Free Energy of Sublimation
Entropy of Sublimation
Structure
Spectrum
Information
MDL molfile
cif
Structured Data File
Uncertainty
Experimental Error
Range
Standard Deviation

Property in RDF

- <c:OrganicMolecule rdf:about="file:///storage/ba8efc2ce0edada69d63b02d1b8630c6.rdf">
- <c:has-inchi>1.12Beta/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>

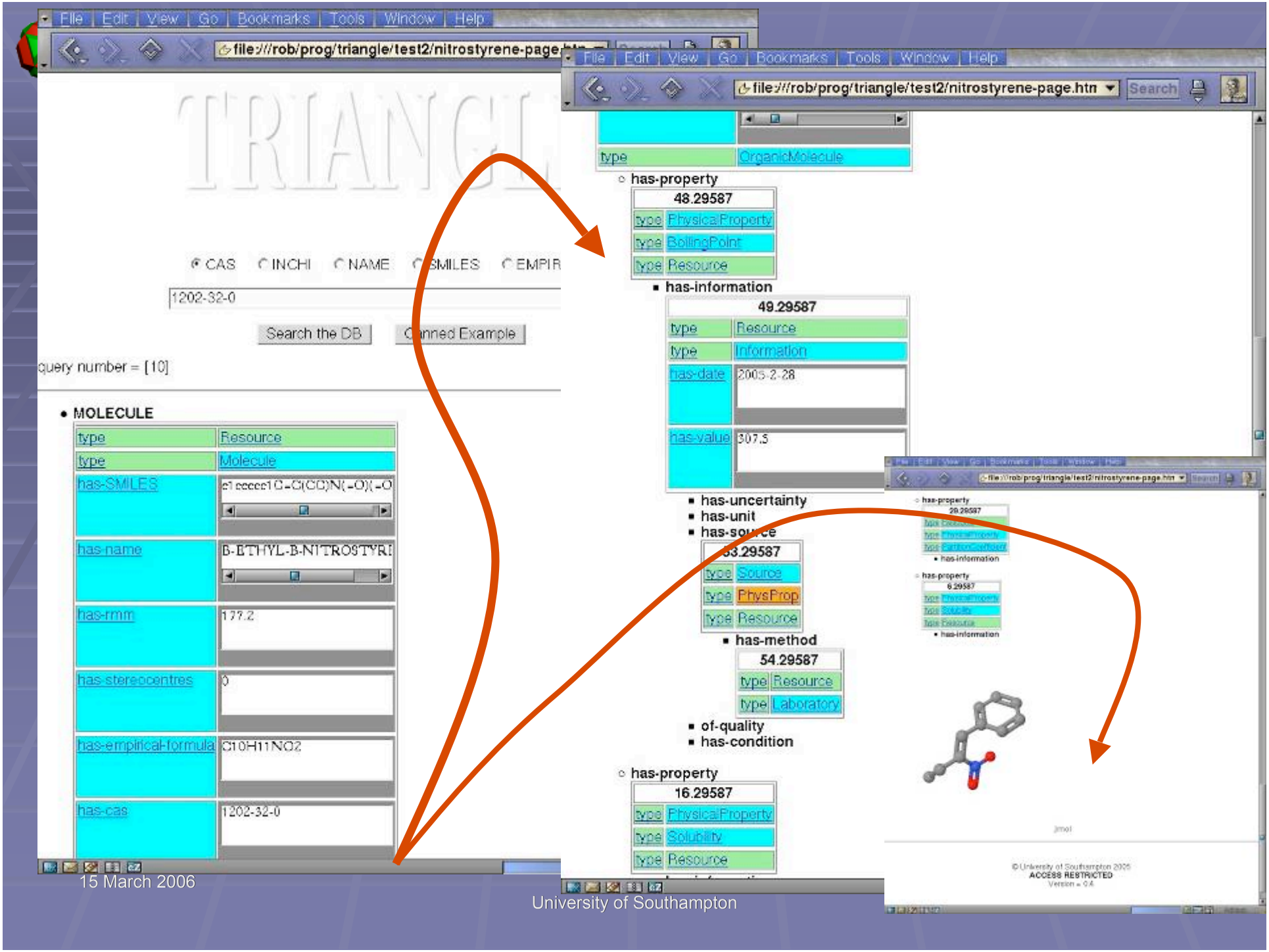
Schema

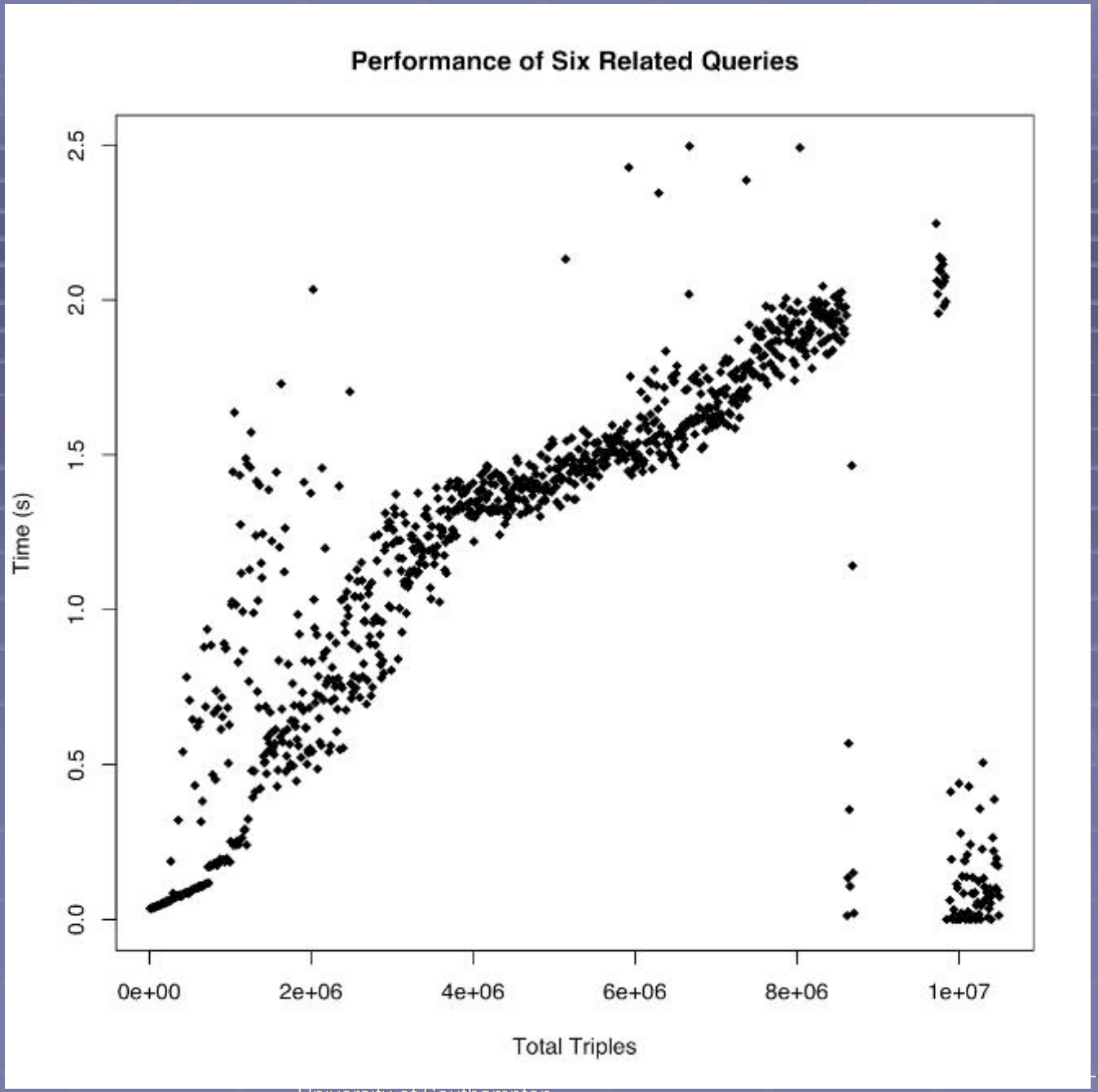
- <rdfs:Class rdf:about="&c;OrganicMolecule">
- <rdfs:label>Organic Molecule</rdfs:label>
- <rdfs:subClassOf rdf:resource="&c;Molecule" />
- </rdfs:Class>

- <rdfs:Class rdf:about="&c;PhysicalProperty">
- <rdfs:label>Property</rdfs:label>
- </rdfs:Class>

- <rdfs:Class rdf:about="&c;PartitionCoefficient">
- <rdfs:label>Paritition 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>

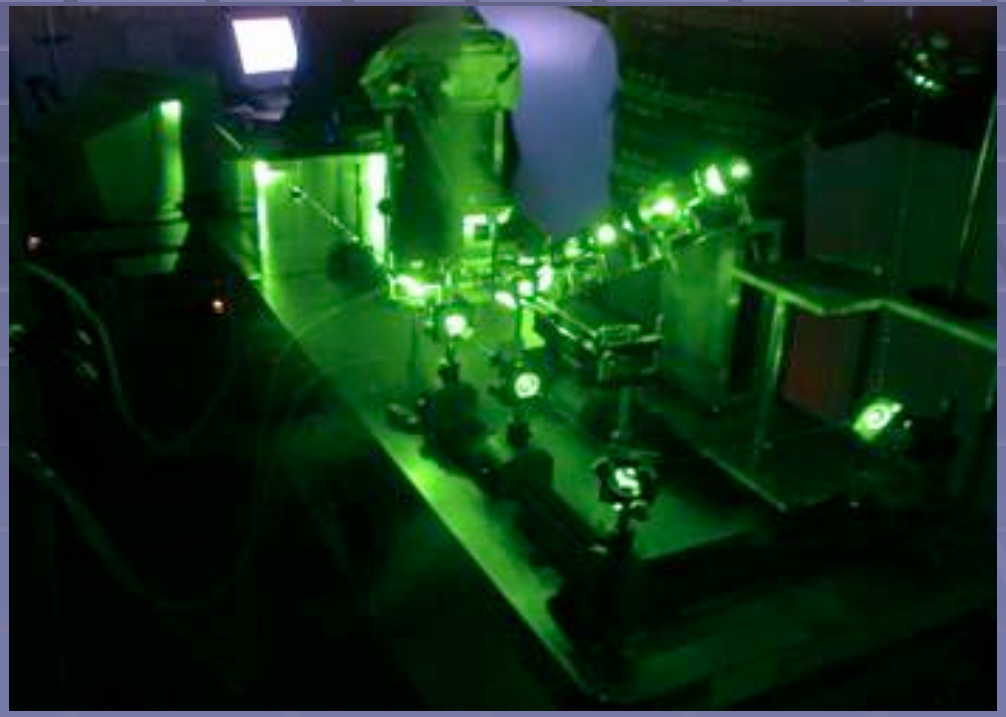
This turns out to be a very flexible approach

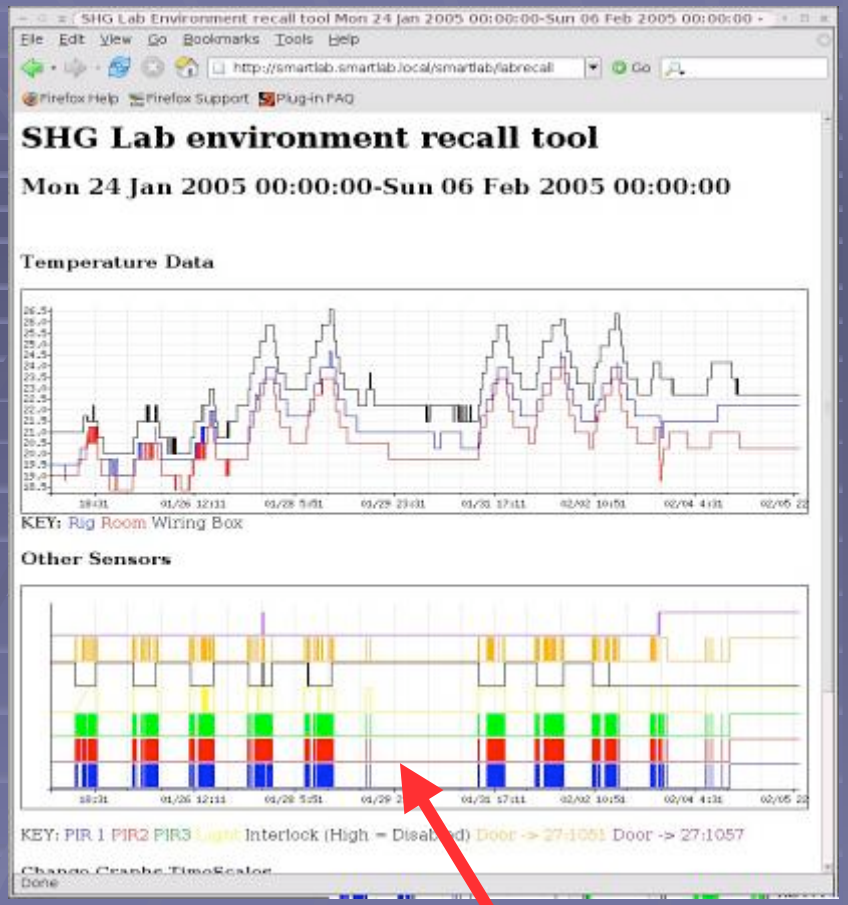

File Edit View Go Bookmarks Tools Window Help
file:///rob/prog/triangle/test2/nitrostyrene-page.htm
TRIANGLE
CAS INCHI NAME SMILES EMPIR
1202-32-0
Search the DB
Canned Example
query number = [10]
MOLECULE
type Resource
type Molecule
has-SMILES
has-name
B-ETHYL-B-NITROSTYRE
has-rmm 177.2
has-stereocentres 0
has-empirical-formula C10H11NO2
has-cas 1202-32-0
type OrganicMolecule
has-property
48.29587
type PhysicalProperty
type BoilingPoint
type Resource
has-information
49.29587
type Resource
type Information
has-date 2005-2-28
has-value 307.5
has-uncertainty
has-unit
has-source
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
ACCESS RESTRICTED


Performance of Six Related Queries
Time (s)
0.0
0.5
1.0
1.5
2.0
2.5
0e+00
2e+06
4e+06
6e+06
8e+06
1e+07
Total Triples

Adapt SHG lab

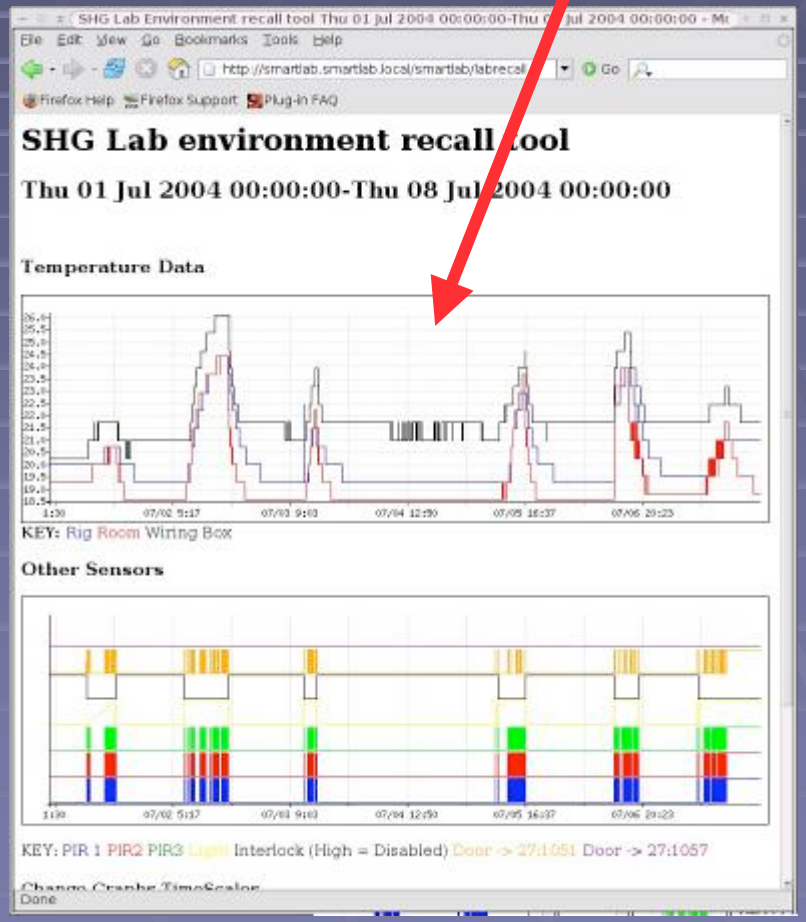
- Capture information from places you would not want to put your eyes



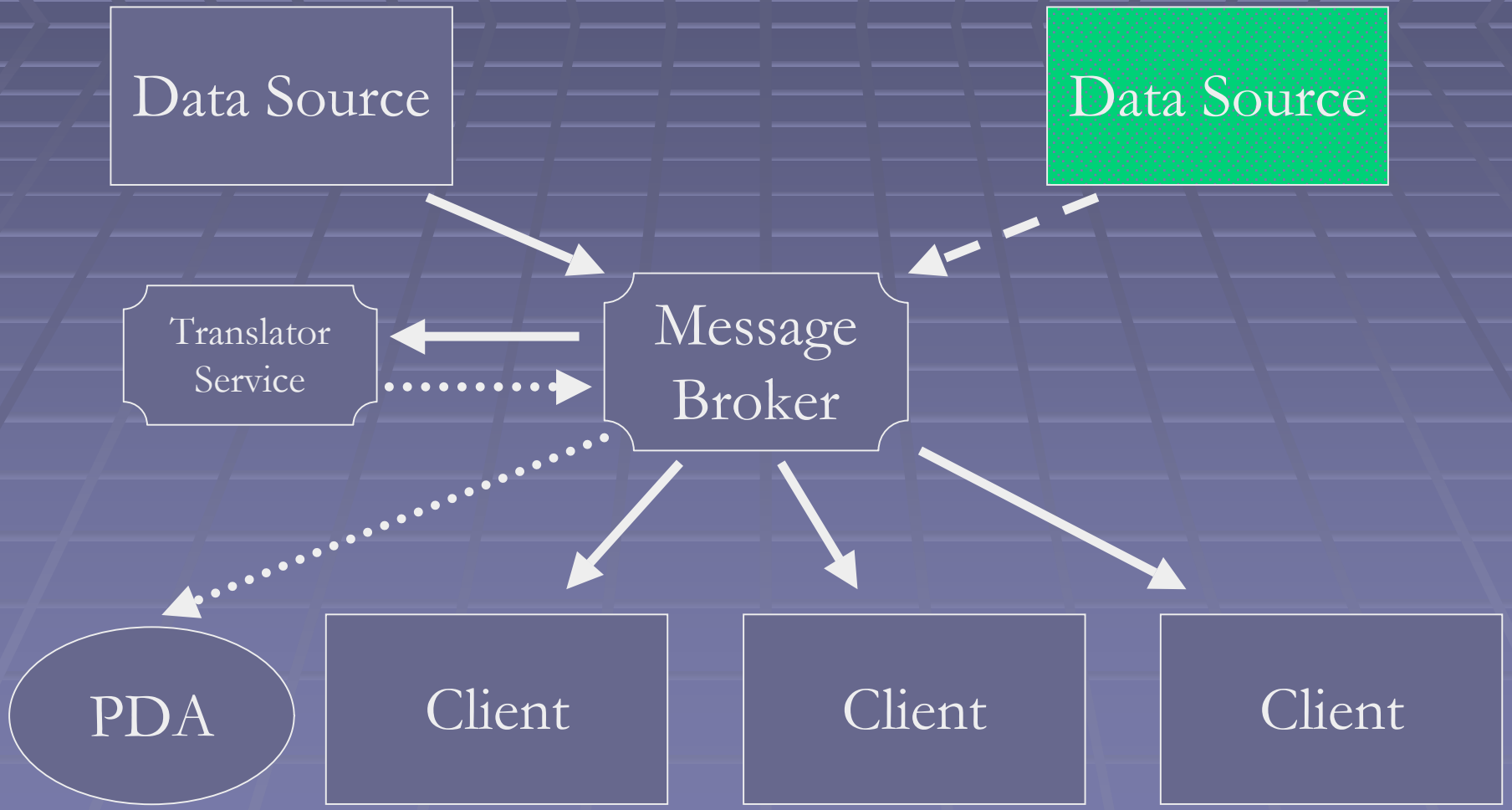


Air Conditioning failed

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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By Jo Twist
BBC News scien

A blend of m
and award-w
is letting scie
escape the la

The software,
"middleware",
computer syst
other securely
instantaneous

As part of a n
project in the
used to let Sc
University che
experiment co
mobiles.

Sensors in the
changes in th
the system ca

"It replaces th

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experiment in more detail.

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.

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

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