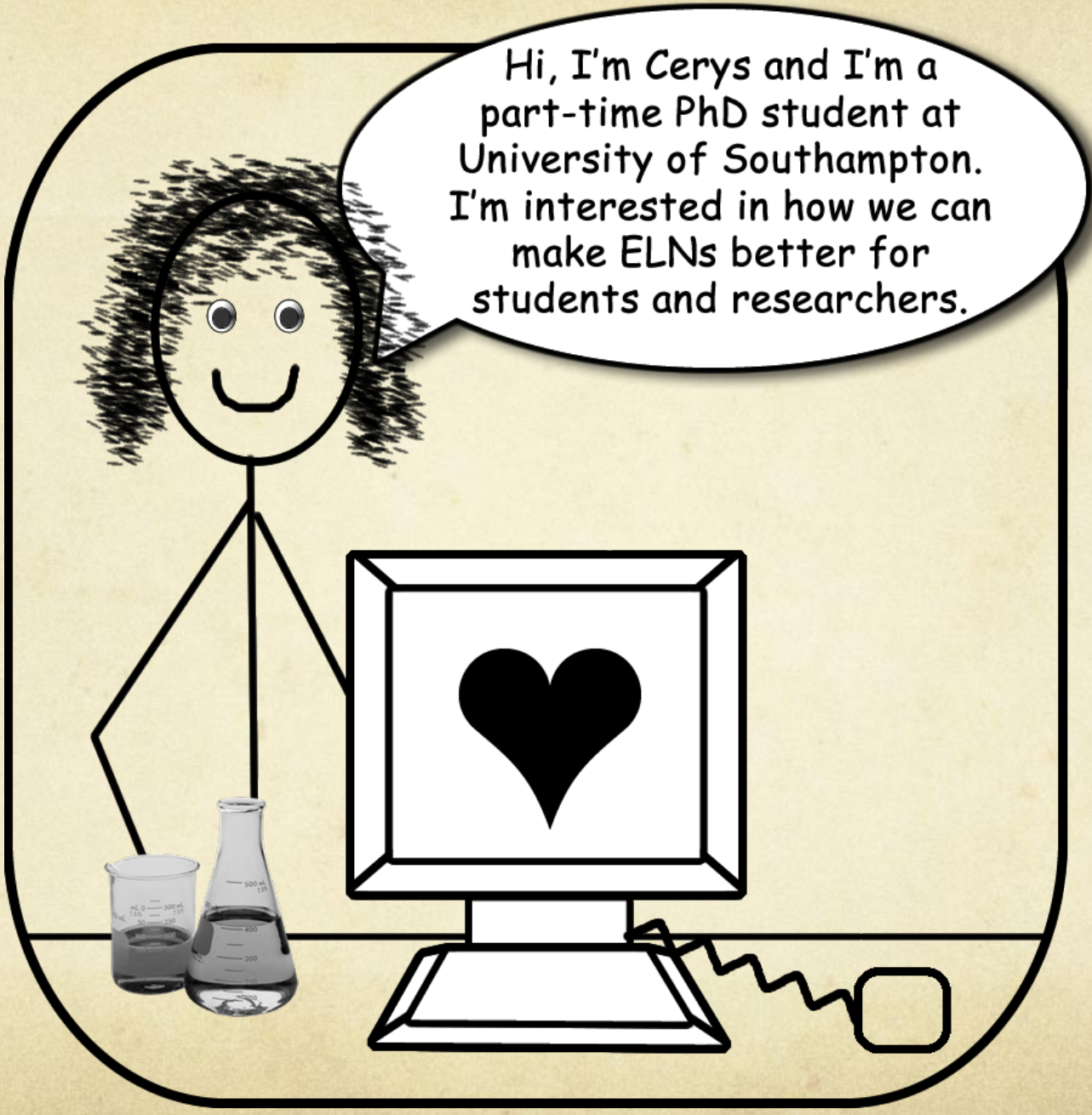
ELNs for researchers and students

A user perspective on ELNs in academic environments


Hi, I'm Cerys and I'm a part-time PhD student at University of Southampton. I'm interested in how we can make ELNs better for students and researchers.

LabTrove

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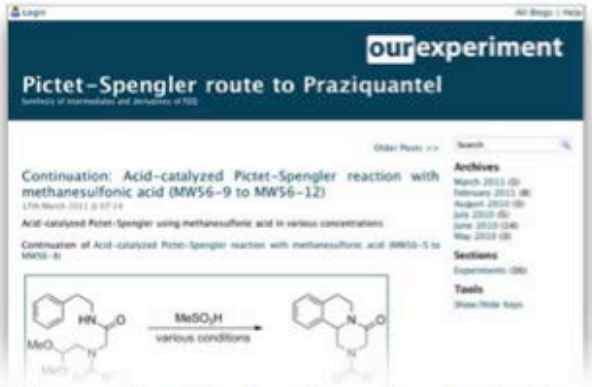


LabTrove enables the formation of a Smart Research

LabTrove
labtrove

labtrove Public Blog Post: Synthesis of amine-linked analogue of TCMDC-123812 via reductive aminatio... http://t.co/Bla5hWbb #malaria #drugdesign
yesterday · reply · retweet · favorite

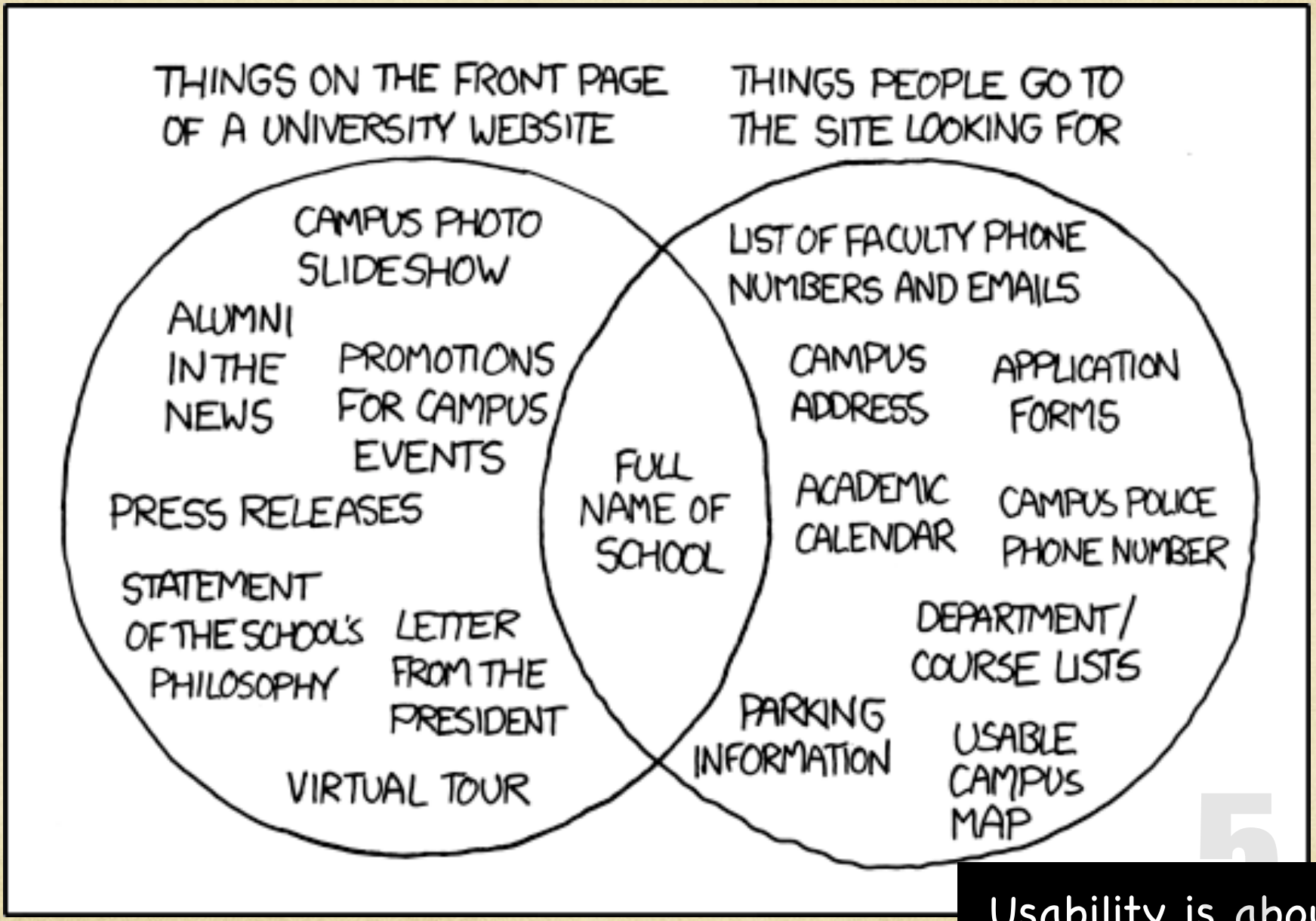
labtrove Public Blog Post: Synthesis of ether-linked analogue of TCMDC-123812 (PMY 37-1) http://t.co/XhqyRb8i #malaria #drugdesign
yesterday · reply · retweet · favorite

labtrove Public Blog Post: Synthesis of 2-Ethoxycarbonylthiolan-3-one http://t.co/m9mU8QKS #malaria

http://www.labtrove.org

Agenda

- A quick overview of usability considerations for ELNs
- Benefits of using ELNs for academic institutions
- Barriers to ELN use
- ELNs and capturing the right information



https://xkcd.com/773/

Usability is about user goals

And making things easy to use!

Different users have different needs

Undergraduates

Researchers

Supervisors

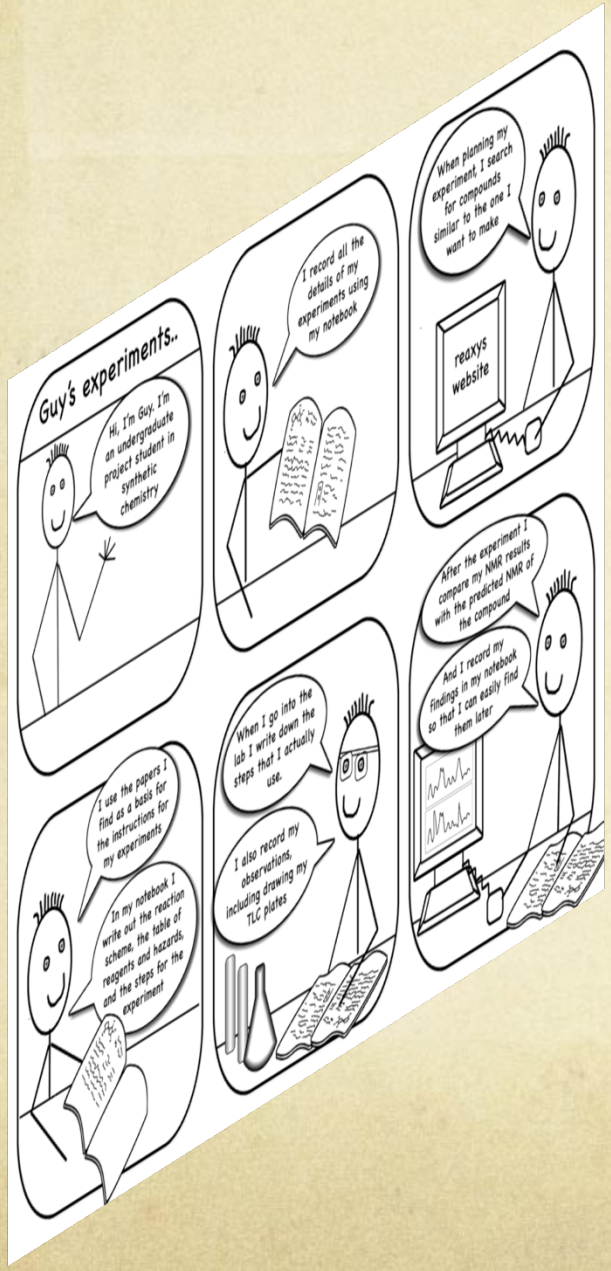
Who else might have needs?

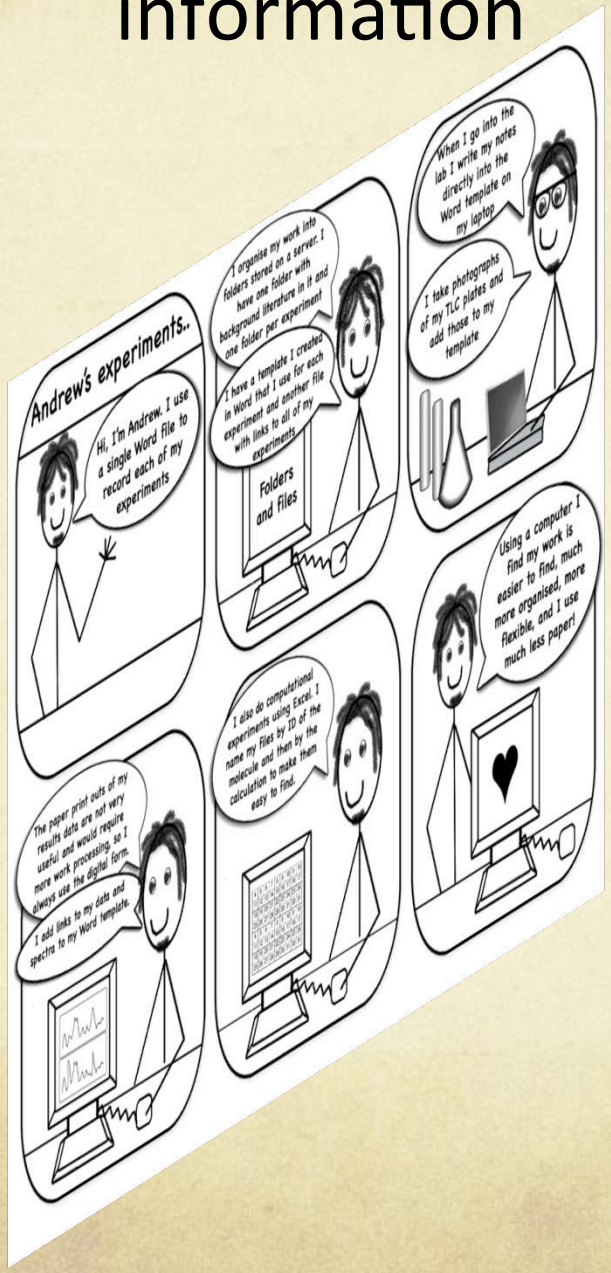
Project funders

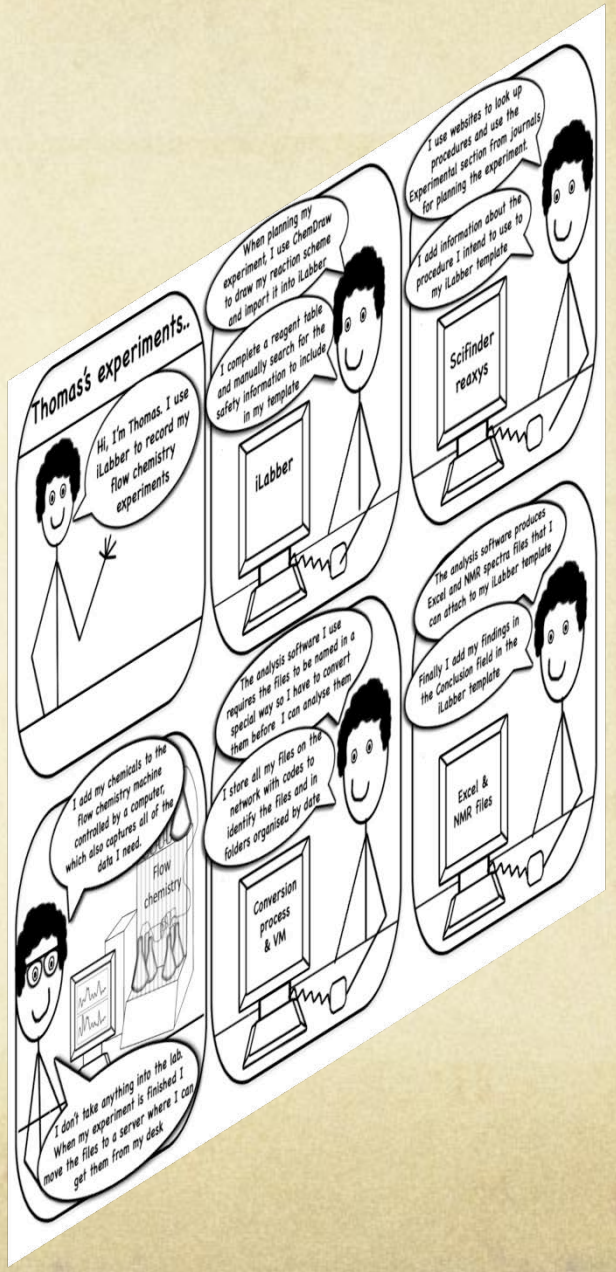
Collaborators

Future students

Different ways of organising experimental information

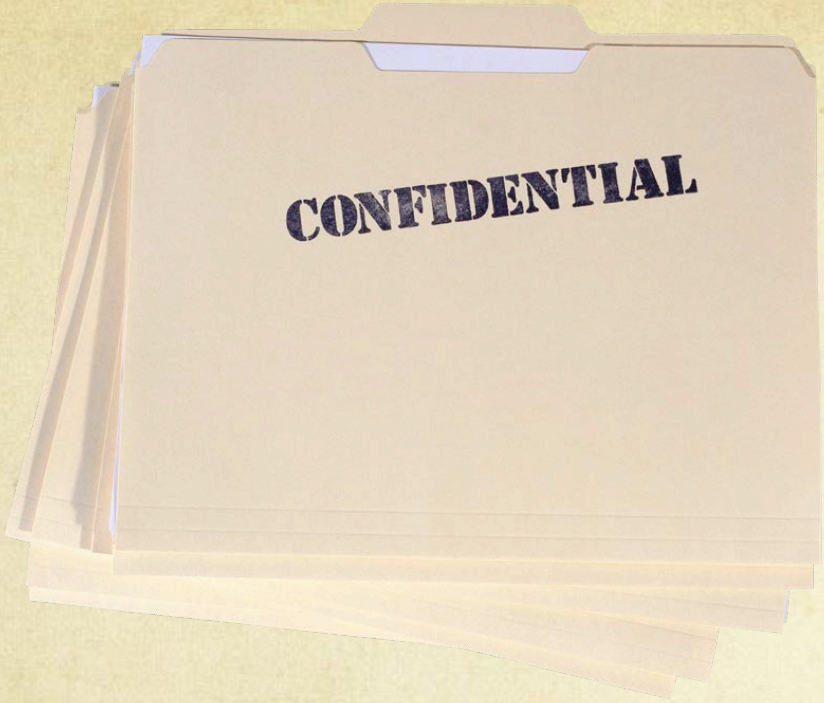






Benefits to using ELNs in academic institutions

What matters to users?



Access

Access to past experiment information and search

Communication!

For when you can't meet face-to-face, but also facilitates communication when you do.

BlogMyData Project - Godiva

Current user: Andrew Milsted | Log Out — All Blogs | Help

BlogMyData

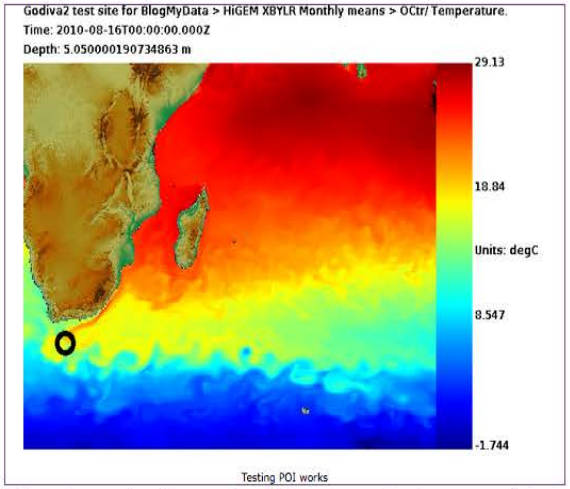
HiGEM Blog

Blog for the HiGEM community

Testing POI works

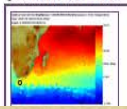
27th August 2010 @ 13:40

Viztype: staticMapWithPoint
Regionofinterest: POINT((21.794815 -38.095867))
Dataset: HIGEM_XBYLR_MONTHLYMEAN
Variableid: temp
Conventions: CF-1.4
Variablestandardname: OCtr/ Temperature.
Variableunits: degC
Bbox: POLYGON((13.359375 -55.689785,95.625 -55.689785,95.625 8.580235,13.359375 8.580235,13.359375 -55.689785))
Crs: EPSG:4326
Time: 2010-08-16T00:00:00.000Z
Calendarsystem: 360_day
Elevation: 5.050000190734863
Elevationunits: m
Elevationpositive: down



ReSC aims to promote e-Science methods in the environmental science community by developing demonstrator projects with collaborators in academia, government agencies (e.g. the Met Office) and industry. These projects will showcase the great potential of e-Science to be a useful method that environmental scientists in many disciplines can use in their everyday research. Tasks that were previously difficult and time-consuming, such as sharing and working with very large data sets, can be made much more efficient.

Attached Files



Search

This Post
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URI Label
Revisions
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This Blog
New Post
Blog Settings
Timeline View
Exhibit View

Archives
October 2010 (3)
September 2010 (2)
August 2010 (8)

Sections
ahm2007 (13)

Viztype
StaticMap (5)
StaticMapWithPoint (2)
Animation (6)

Dataset
HIGEM XBYLR MONTHLYMEAN (13)

Variablestandardname
OCtr/ Temperature. (6)
OCtr/ Salinity. (2)
Density (5)

Calendarsystem
360 Day (13)

Elevationunits
M (13)

Elevationpositive
Down (13)

Tools
Show/Hide QR Code
Show/Hide Keys

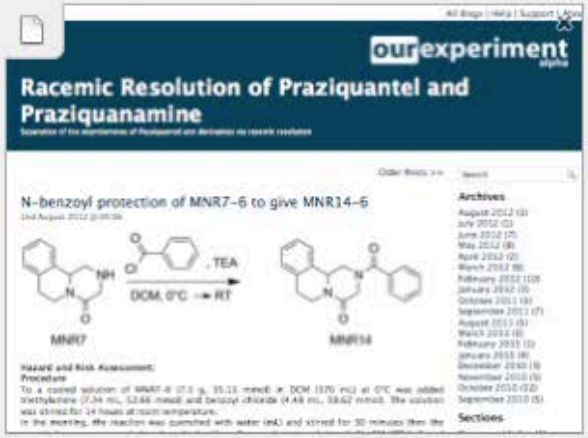
Open Notebooks Mat Todd's PZQ Project

PZQ

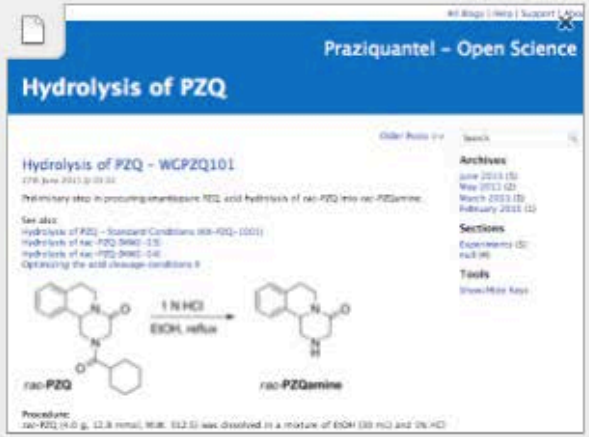
Praziquantel – Open Science

Pictet–Spengler route to Praziquantel

Racemization of PZQ and PZQamine



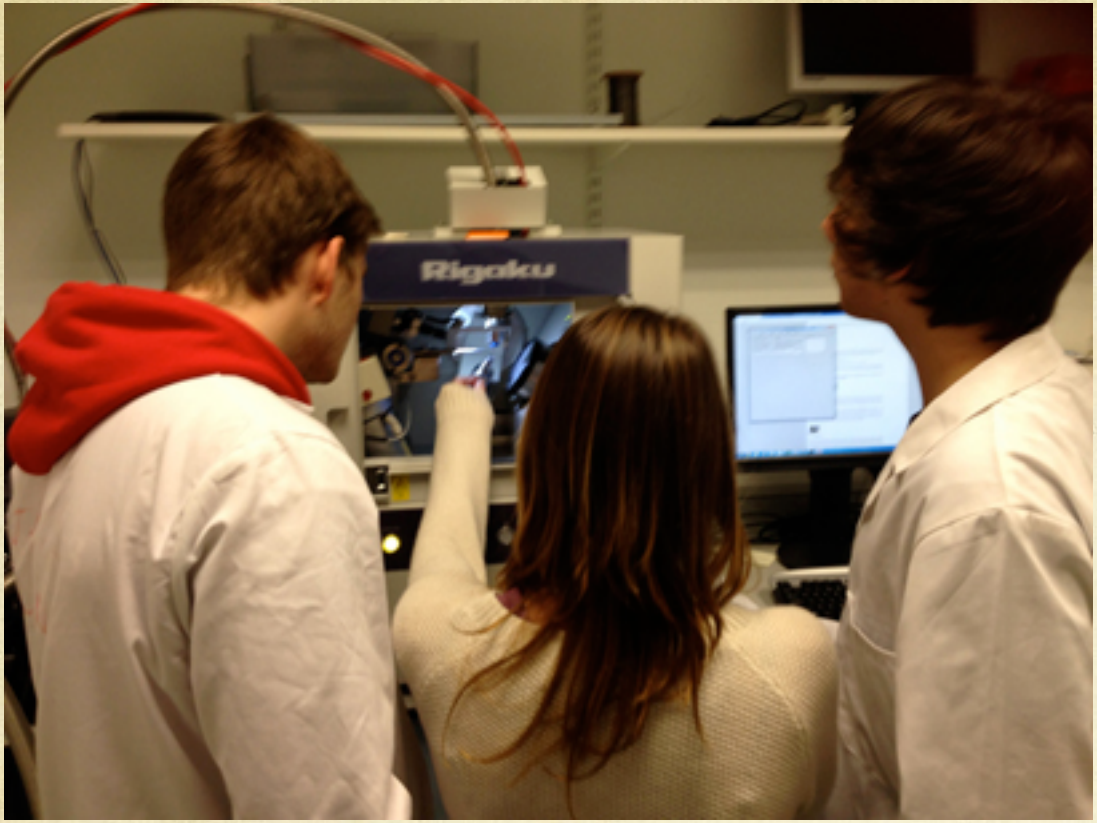
Racemic Resolution of Praziquantel and



Hydrolysis of PZQ

Introduction

Open access is controversial but has real benefits for some



Students

Training and standards

Tpp Methyl ester Hydrolysis:- Methord 2

9th April 2009 @ 16:50

Lab Note Book Or Experiment Code: FDH-5405-E7P26
Post Type: Methord_2
Procedural Step: Methord_2
Date Of Experiment: 27-11-08
Experiment Name: Tpp_Methyl_ester_Hydrolysis
Experiment Code:FDH/5405/E7P26
Date of Experiment:27/11/08

- reaction mixture added to 100ml of DCM
- solid formed...disolved in DCM/MeOH + water and evaporated to near dryness
- re desolved in 200ml choroform+20ml meOH, sonicated most desolved.
- 3oml water added mysells leeding to sold problems and poor seperation seen.
- 100ml water added now gives clear layer with mysells below
- transfered to bigger 500ml sep funnle.

this picture taken directly after transferance

- aprox. 30ml 2Mhydrocloric added to give emitate seperation. and turn porphyrin protenated green.
- much bettter behavd now....loverly shade of green too.

protonated prophyrin with 2M HCL

- HCL reextracted with 100ml CHCl3.
- fluffly brown noted between interface. contaminant?
- organic rinced5 times 100ml water. first rinc turns it back to puple

now purple organic with aqueous

- water re-extracted into chloroform 100ml and rince 5 times h2o.
- organicfractions combined and dryed over anhydrous sodium sulfate

27-11-08 (2)
30-11-08-1-12-08 (1)

Experiment Name

Prepartation Of Fulleropyrrolidin Alcohol:-Planning And Saftey (8)
Preparation Of N-Glycine (amino-Ethoxy-Ethanol) Tert Butyl Acetate (4)
Preparation Of P-tert Butly (bis[cyanomethoxy)dihydroxy]) Calix (2)
Preperation Of Mono Para Methyl Ester Meta Tetra Phenyl Porphyrin (10)
Removal Of A Protecting Group To Give [(hydroxyethoxy)ethyl Amino] Acetic Acid Repeat Ed (2) (4)
Removal Of A Protecting Group To Give [(hydroxyethoxy)ethyl Amino] Acetic Acid (5)
Prepartation Of Fulleropyrrolidin Alcohol (repeat 2) (3)
Prepartation Of Fulleropyrrolidin Alcohol (repeat 2) (1)
Tpp Methyl Ester Hydrolysis (5)

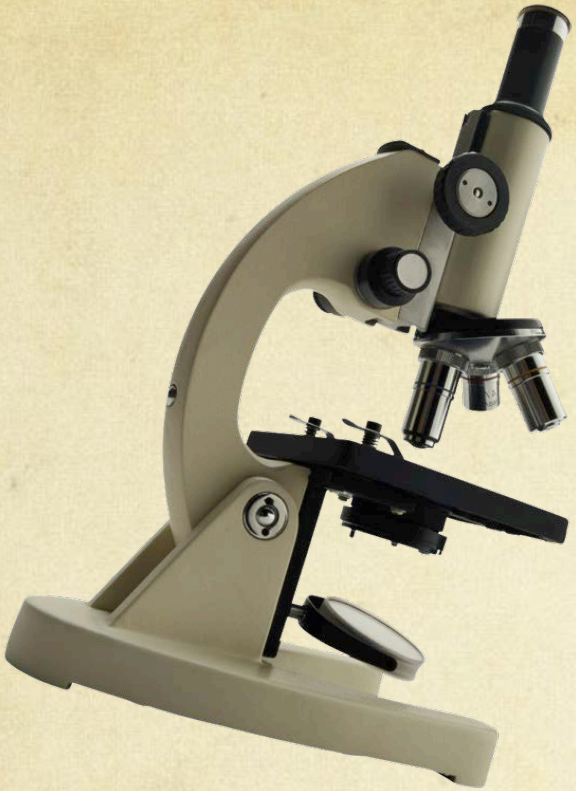
Chemical

Dichloromethane (1)
Triethylamine (1)
2-(2-Aminoethoxy)ethanol (1)
Template (1)
TertButylbromoacetate (1)
Tert Butyl 2 (2 (2 Hydroxyethoxy)ethylamino)acetate (1)
SodiumHydroxide1M (1)
Buckminsterfullerene (1)
Paraformaldehyde (1)
Toluene (1)
2-(2-(2-hydroxyethoxy)ethylamino)acetic Acid (1)
Fulleropyrrolidin Alcohol (1)
Pyrrole (1)
Methyl4-formylbenzoate (1)
Benzaldehyde (1)
Chloroform (1)
BoronTrifluorideEtherate (1)
2,3-Dichloro-5,6 Dicyano-1,4-Benzoquinone (1)
5-4-Methyl Benzoate
10,15,20-tri Phenyl Porphyrin

Support for students with disabilities

Undergraduate Advanced Crystallography Trial

Attitudes towards ELNs



Data

Provenance & Citations

DOI's for Data

LabTrove

Reports

(3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

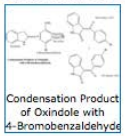
Graham Tizzard, Nicola Knight
13th June 20[illegible]3 | doi:10.5258/poc/lt/r/1

This Report
Print view

Availability
Currently:
Public (Googleable)
Make:
Private (Just For You)
Notebook Users only

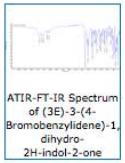
Condensation Product of Oxindole with 4-Bromobenzaldehyde

Substituent: Bromo



ATIR-FT-IR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

Spectroscopic Method: ATIR-FT-IR
Substituent: Bromo
ATIR-FT-IR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

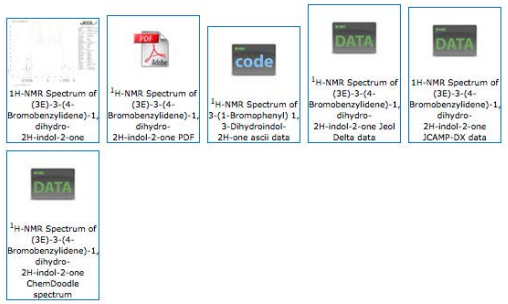


Interpretation of ATIR-FT-IR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one:

ATIRFT-IR Wave Number (cm^{-1})	Assignment	Remarks
3141	N-H stretching vibration (ν(N-H) (1° amide)	Symmetrical stretching vibrations of the NH group
3077	Aromatic C-H stretching vibration (ν(C-H)	C-H aromatic stretching in the region 3100-3000cm^{-1}
3024	Aryl-H	Often obscured and appears on the region 3010-3040cm^{-1}
2898	C-H stretching vibration	Saturated C-H stretching at the region 2840-2930cm^{-1}
1700	C=O stretching vibration	Attributed to the carbonyl functional group and

^{1}H-NMR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

Spectroscopic Method: H-NMR
Substituent: Bromo
^{1}H-NMR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

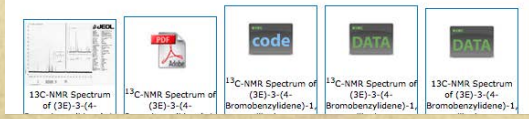


Interpretation of ^{1}H-NMR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one:

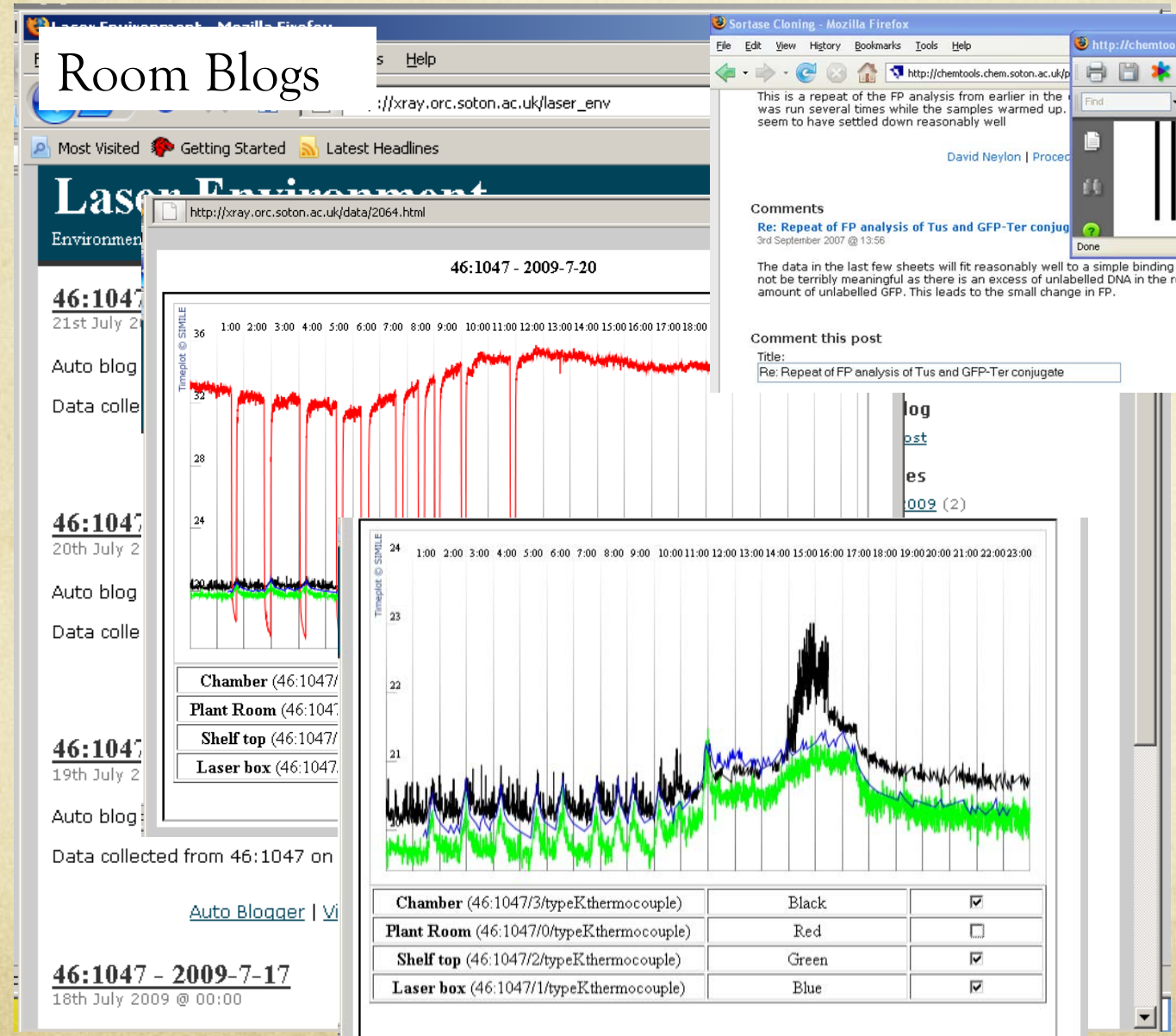
Chemical Shift, ppm	Multiplicity, (n+1)	Coupling Constant, J Hz	Integration, Σ H	Inference
1.62				$CDCl_3$
6.85 - 6.89	multiplet		2	oxindole hydrogens on C_5 and C_6
7.26 - 7.29	multiplet		2	oxindole hydrogens on C_4 and C_7
7.59 - 7.62	multiplet		4	benzylic hydrogens on C_9, C_{10}, C_{12} and C_{13}
7.72	singlet	n/a	1	vinylic hydrogen on C_8
8.28	broad singlet	n/a	1	amino hydrogen on N_1

^{13}C-NMR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

Spectroscopic Method: C-NMR
Substituent: Bromo
^{13}C-NMR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one



Connecting physical & digital worlds



Automatic data from Matlab

blogs@xray

WSB Matlab Autoblog

Matlab stuff produced by Bill's machine, sometimes with his help.

Older Posts >>

Search

This Blog

New Post

ion_vs_spot.m

14th May 2012 @ 11:59

matlab code:

```
%ion_vs_tspot
% show what happens to the ionizat
clear all
Ep = 5e-6; % pulse energy in joule
tau = 500; % pulse lenght in fs
lambda = 2200e-9;
w = 3:0.5:7; % spot size in um
%now calc intensity
P0 = sqrt(2/pi) * sqrt(2* log(2))
Aeff = (pi * (w/1e6).^2)/2;
I = 1e-4 * P0./Aeff; % in W/cm^2
ion = zeros(size(tau));
cutoff_h = zeros(size(tau));
for ii = 1:length(I)
    [ion(ii) cutoff_h(ii)] = adk8_
end
cutoff_lambda = lambda ./cutoff_h
```

plot

matlab code:

```
figure(30)
%plot(w, ion)
plotyy(w, ion, w, cutoff_lambda*1e9);
xlabel('spot size /um')
ylabel('final ionization level');
title(sprintf('Final ionization level & cutoff wavelength vs spot size, %g uJ puls
%grid on
```

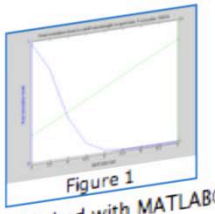


Figure 1

Published with MATLAB® 7.11.1

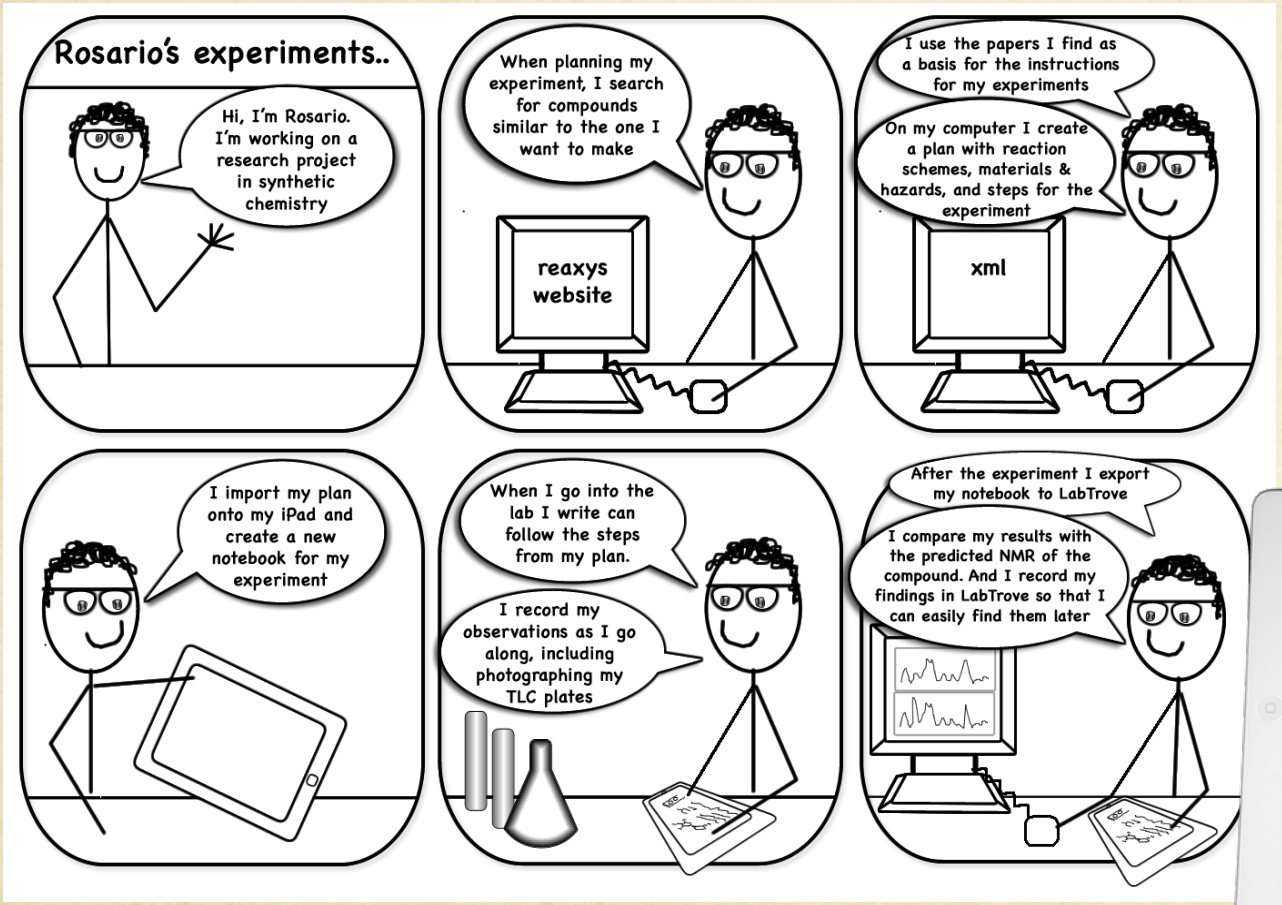
/Volumes/jfDfsResPhysicsAstronomyResearch$/Private/xraylab/grants/2012 OPO HHG

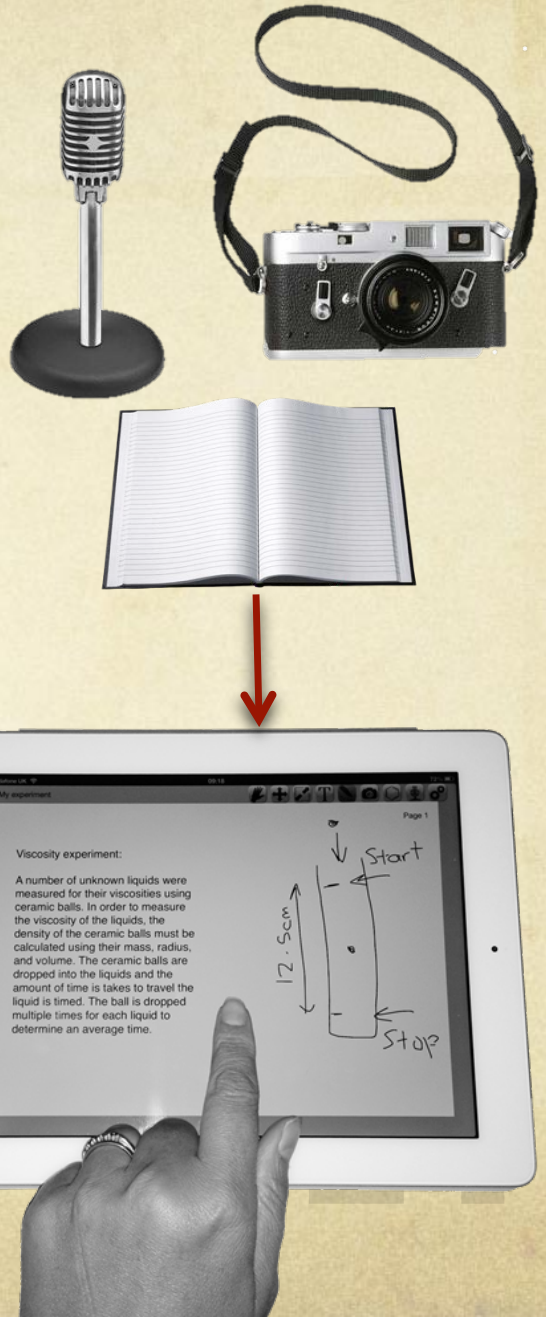
Attached Files

View Source | Matlab Autoblogging | Comments (0)

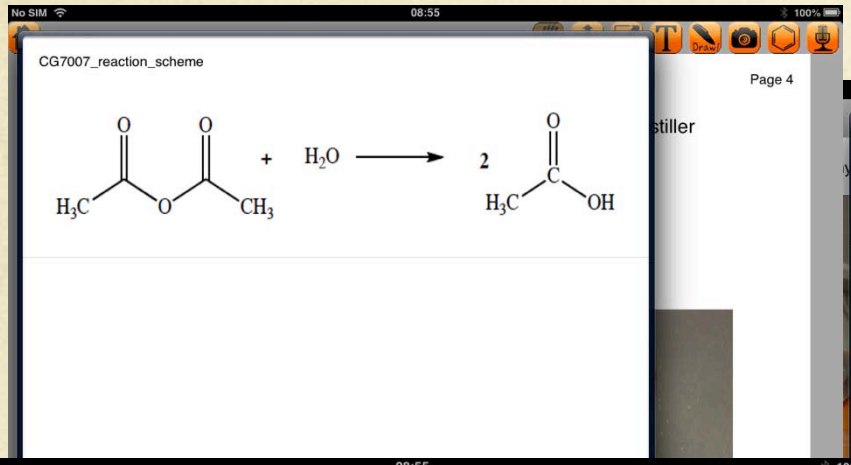
Computational processes can be run and captured

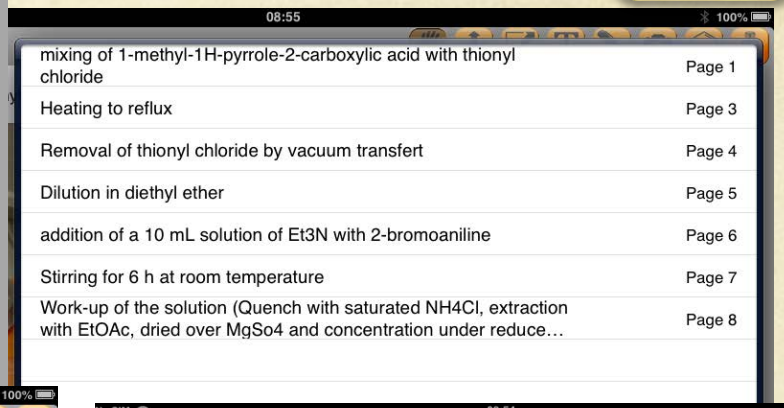
Flexible capture using mobile devices

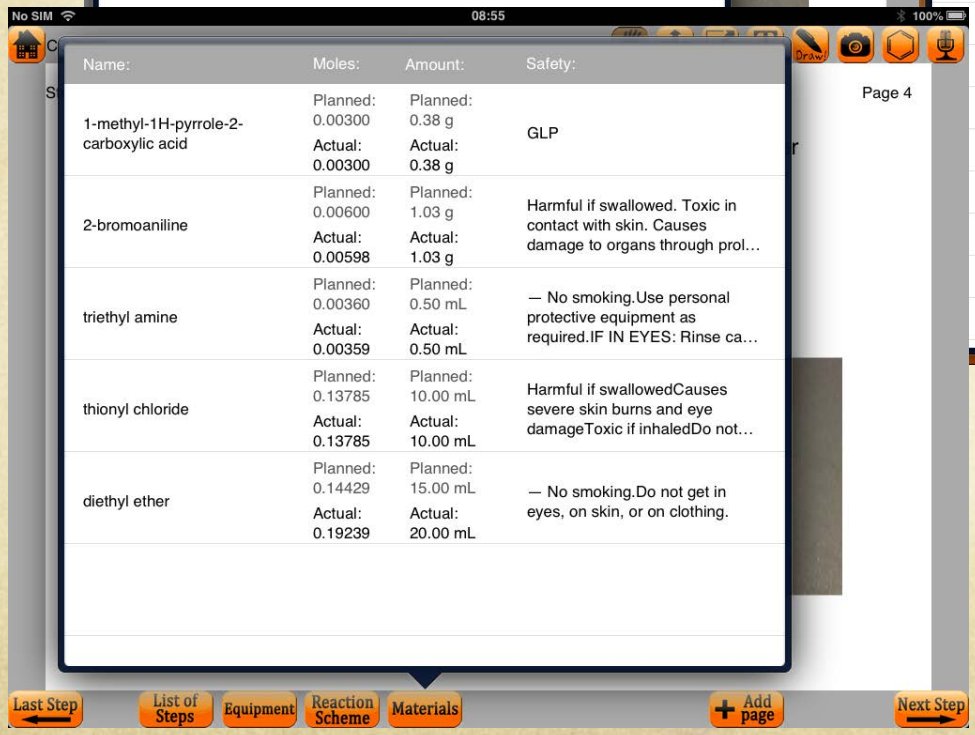


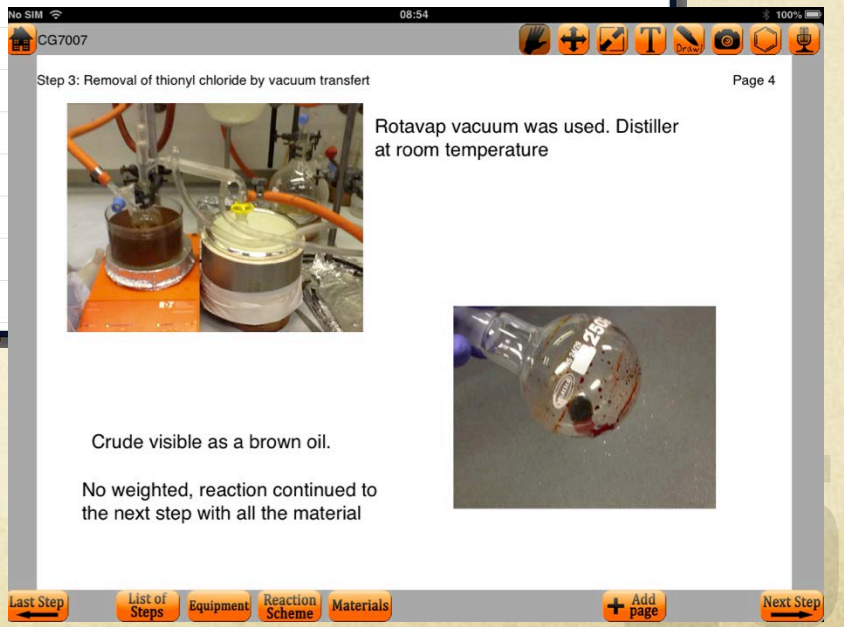


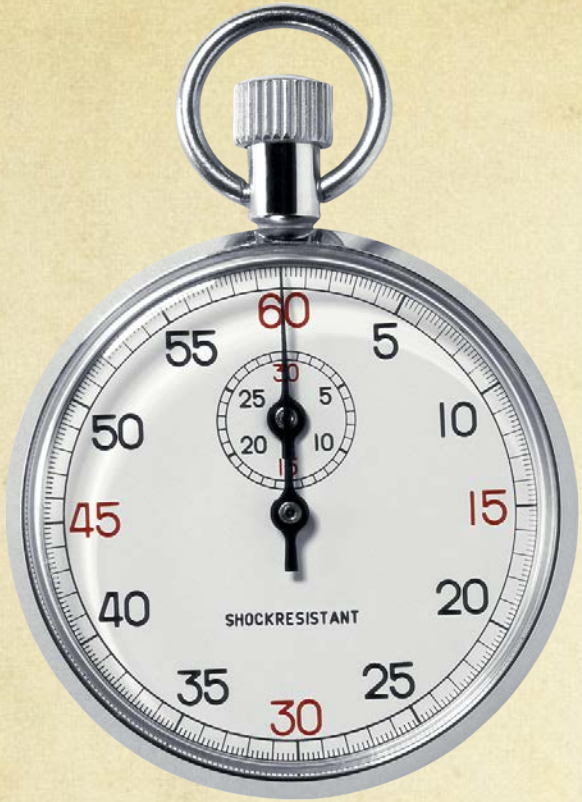
Organic synthesis trial











- Duplicate experiments
- Re-use for reports and theses
- Publication process
- Use of templates
- Encouraging standards across a group

Productivity

Barriers to adoption

Costs

Access

Integration

Data

Anxiety

Note-taking

Anxiety

Bad experiences

"Books don't crash"

Ease of use!

"Writing on paper is better"

Reliability

Additional burden

Note-taking

Doesn't record the right information

Risk of semi-automating note-taking

"Learning to write a paper notebook is an essential part of a PhD student's training"

"Cut and paste culture"

"Loss of observation skills"

Capturing the ‘right’ information about the experiment

ELNs can provide a structured environment for recording information

But is that good or bad?

- Structured
- Provides cues
- Potential problems

Templates

It's not about the procedure..

- What did I do?
- Why did I make that decision?
- What did I see?
- Why do I think that happened?
- How does it relate to my knowledge?
- What might I forget to record that is important?
- Will what I capture help me when I come to look up the experiment in the future?

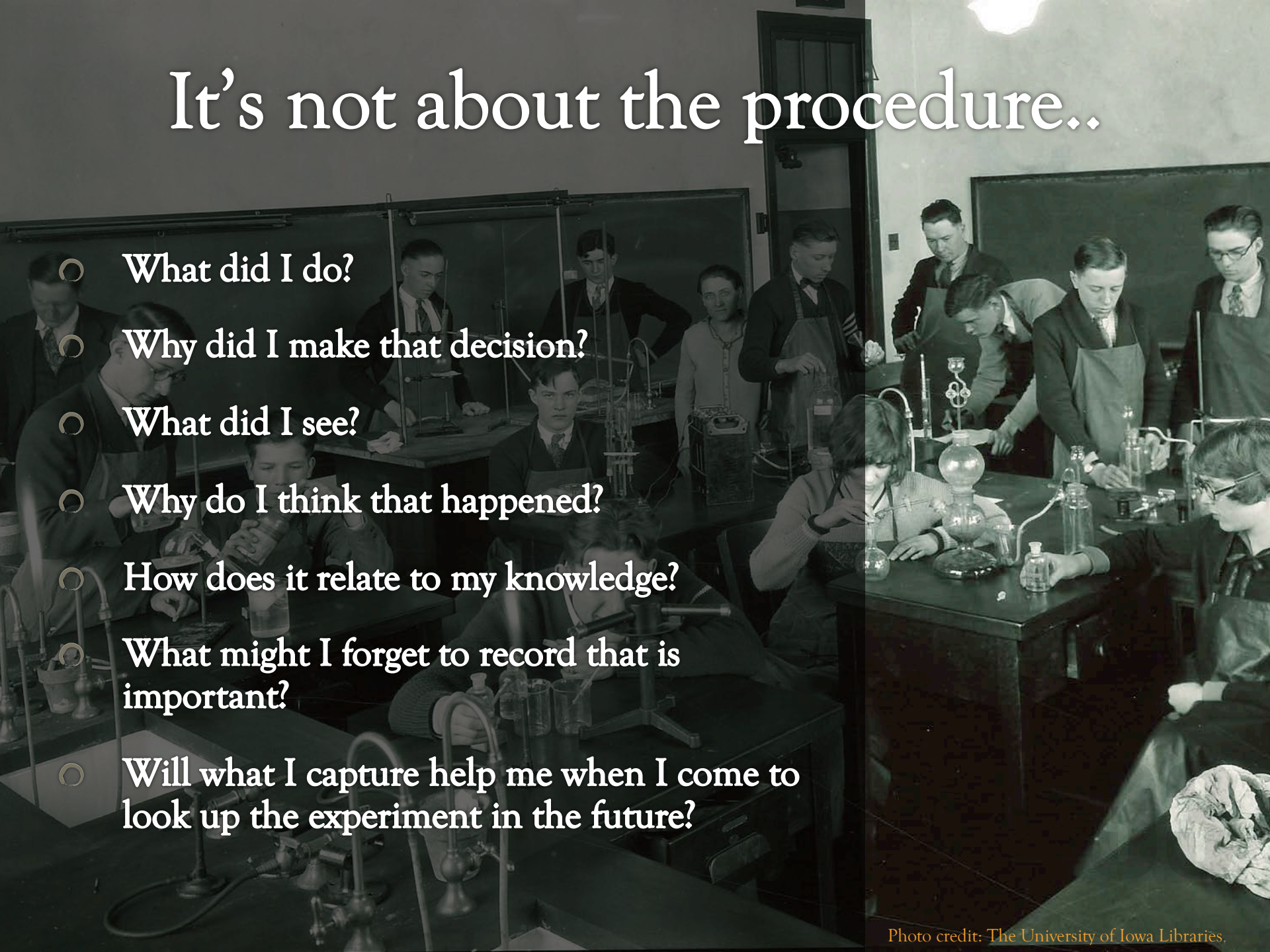


Photo credit: The University of Iowa Libraries.

Post-experiment questionnaires

Template condition

1. Name of experiment
2. Aim of the experiment
3. Balanced equation with relative molecular masses
4. Step-by-step experiment procedure
5. Results
6. Discussion
7. Conclusions

No Template condition

Study findings

Templates

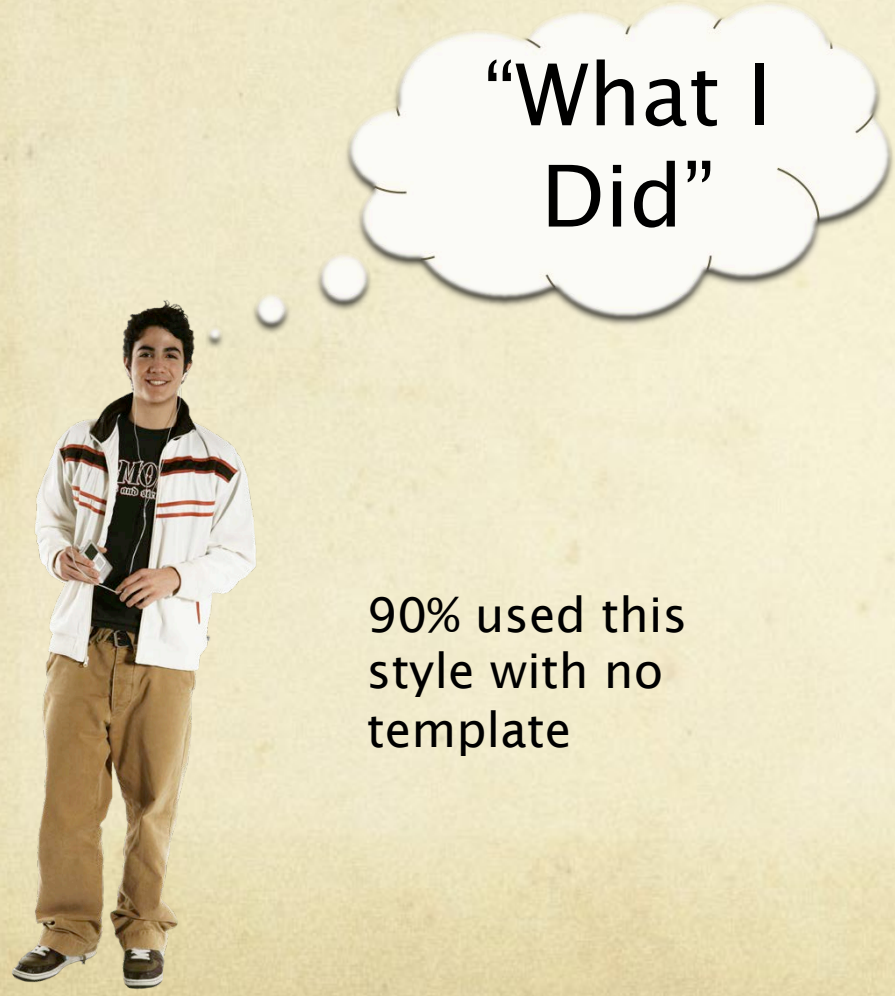
- Give us information we ask for: reaction schemes, RMMs, results, details of the analysis
- Fewer observations and explanations
- Learning and theory

No Templates

- Give more of the personal experience: observations and explanations
- Fewer reaction schemes, no RMMs, fewer results and analysis, much less learning and theory

Unexpected findings

A change in the style of reporting



90% used this style with no template

More than half of those students switched to this style when they used the template

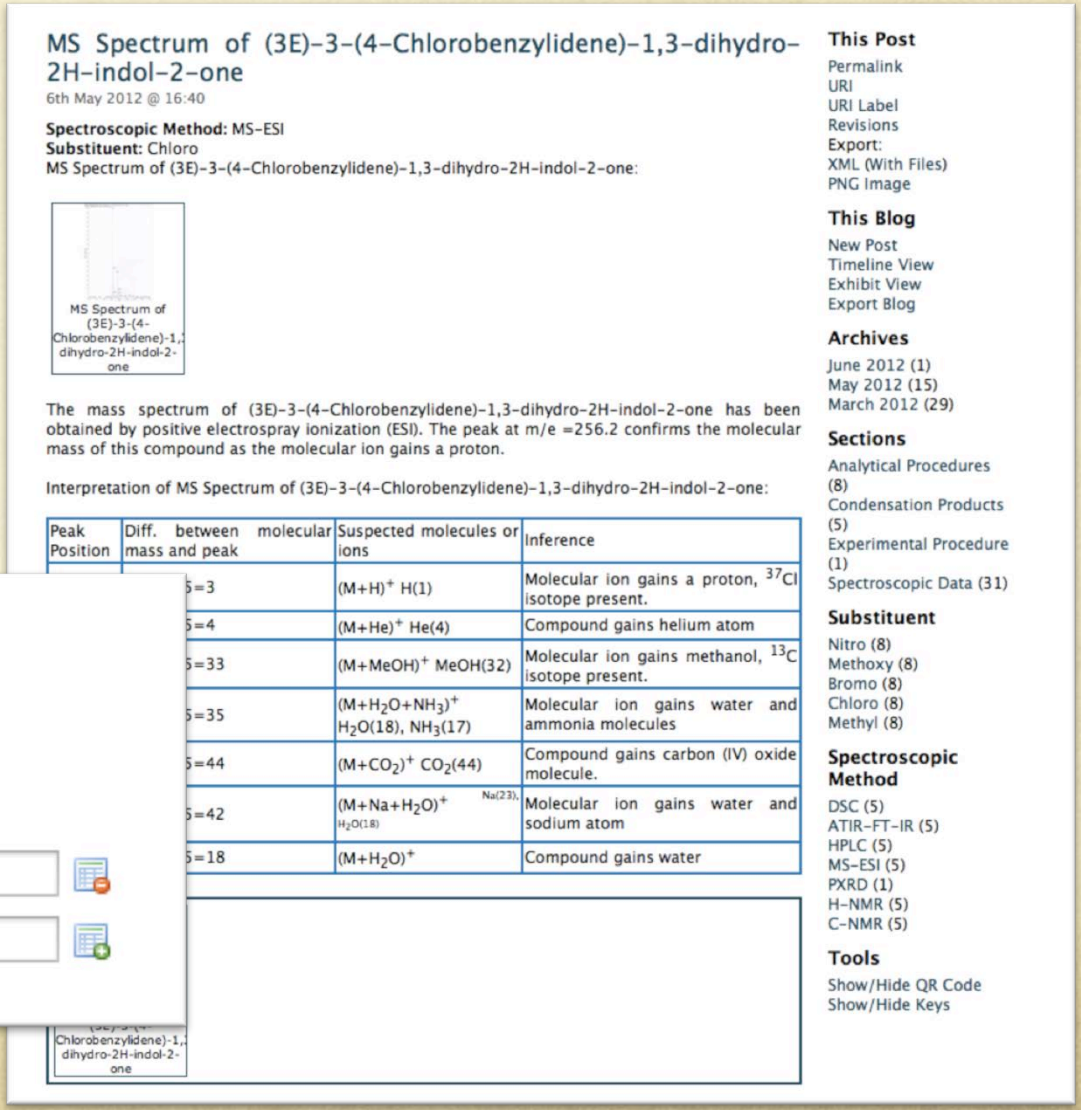
Further investigations..

With different templates and Lego!

Metadata

LabTrove and metadata

Automatic metadata
and
User-defined metadata



MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one

6th May 2012 @ 16:40

Spectroscopic Method: MS-ESI
Substituent: Chloro
MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one:

MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one

The mass spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one has been obtained by positive electrospray ionization (ESI). The peak at m/e =256.2 confirms the molecular mass of this compound as the molecular ion gains a proton.

Interpretation of MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one:

Peak Position	Diff. between molecular mass and peak	Suspected molecules or ions	Inference
	=3	$(M+H)^+$ H(1)	Molecular ion gains a proton, ^{37}Cl isotope present.
	=4	$(M+He)^+$ He(4)	Compound gains helium atom
	=33	$(M+MeOH)^+$ MeOH(32)	Molecular ion gains methanol, ^{13}C isotope present.
	=35	$(M+H_2O+NH_3)^+$ $H_2O(18)$, $NH_3(17)$	Molecular ion gains water and ammonia molecules
	=44	$(M+CO_2)^+$ $CO_2(44)$	Compound gains carbon (IV) oxide molecule.
	=42	$(M+Na+H_2O)^+$ Na(23), $H_2O(18)$	Molecular ion gains water and sodium atom
	=18	$(M+H_2O)^+$	Compound gains water

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URI
URI Label
Revisions
Export:
XML (With Files)
PNG Image

This Blog
New Post
Timeline View
Exhibit View
Export Blog

Archives
June 2012 (1)
May 2012 (15)
March 2012 (29)

Sections
Analytical Procedures (8)
Condensation Products (5)
Experimental Procedure (1)
Spectroscopic Data (31)

Substituent
Nitro (8)
Methoxy (8)
Bromo (8)
Chloro (8)
Methyl (8)

Spectroscopic Method
DSC (5)
ATIR-FT-IR (5)
HPLC (5)
MS-ESI (5)
PXRD (1)
H-NMR (5)
C-NMR (5)

Tools
Show/Hide QR Code
Show/Hide Keys

Section*

Analytical Procedures

Metadata

key	value
Substituent	Nitro
Spectroscopic	DSC

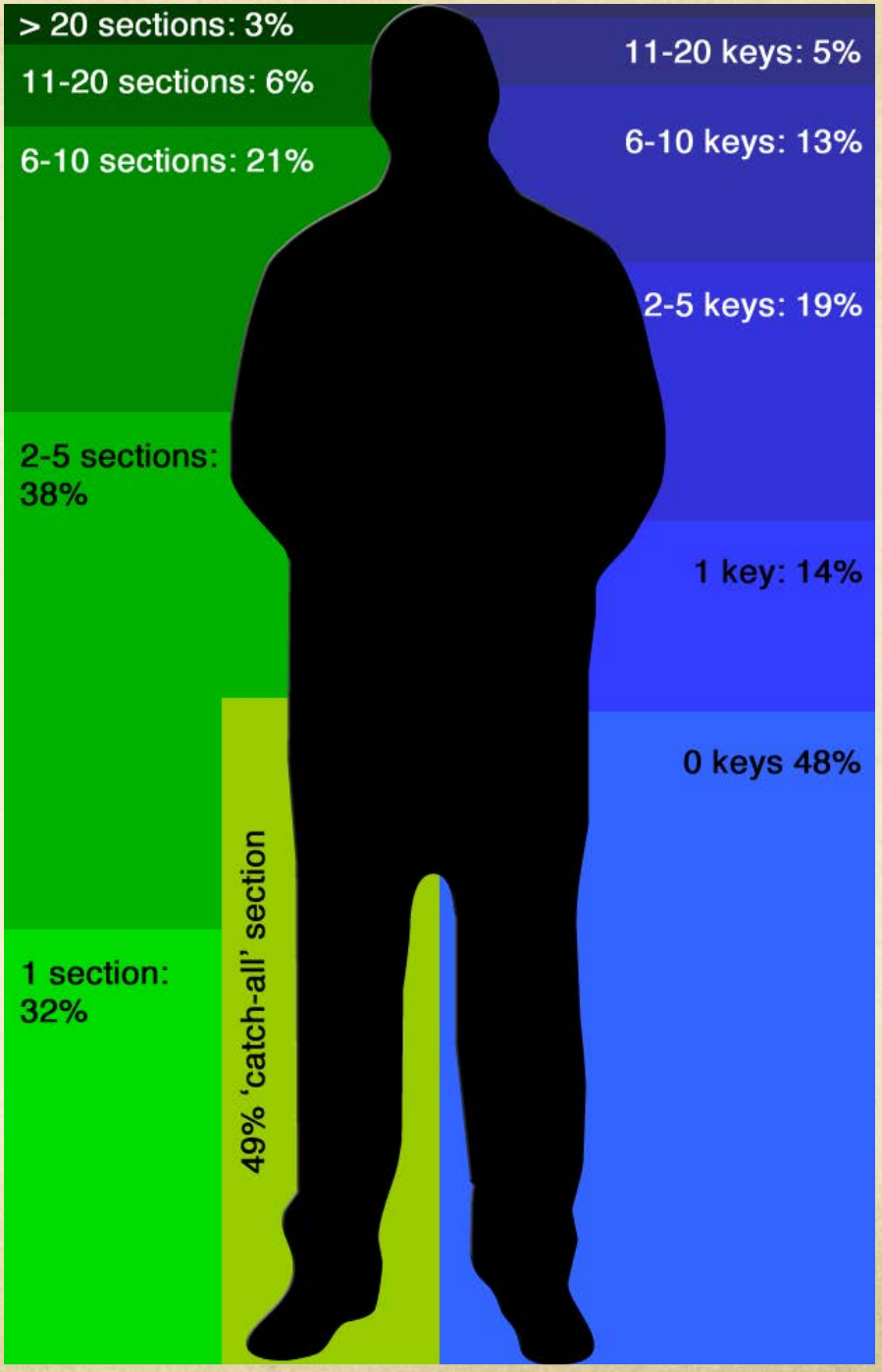
Metadata Survey

104 notebooks

A big proportion of our users are not really adding metadata!

Metadata anxiety

- ‘Blank canvas’ effect
- Consistency
- Duplication
- Mistakes
- Inappropriate metadata



What did we learn?

- Metadata has to be present to be useful!
- Common mistakes and “sense-making”
- Tells us about the interests and needs of the communities
- Users will use predefined values if they are available
- A number of possible strategies to encourage better use (and user experience) of metadata in ELNs

Further research..

What are the right questions ?

Summary

- For ELNs to be useful they need to match the needs of users
- ELNs can bring benefits in academic environment
- But barriers to adoption need to be overcome
- Templates can be used to help enforce standards and produce high quality records but care is needed
- Strategies are needed to encourage better metadata use and curation by researchers