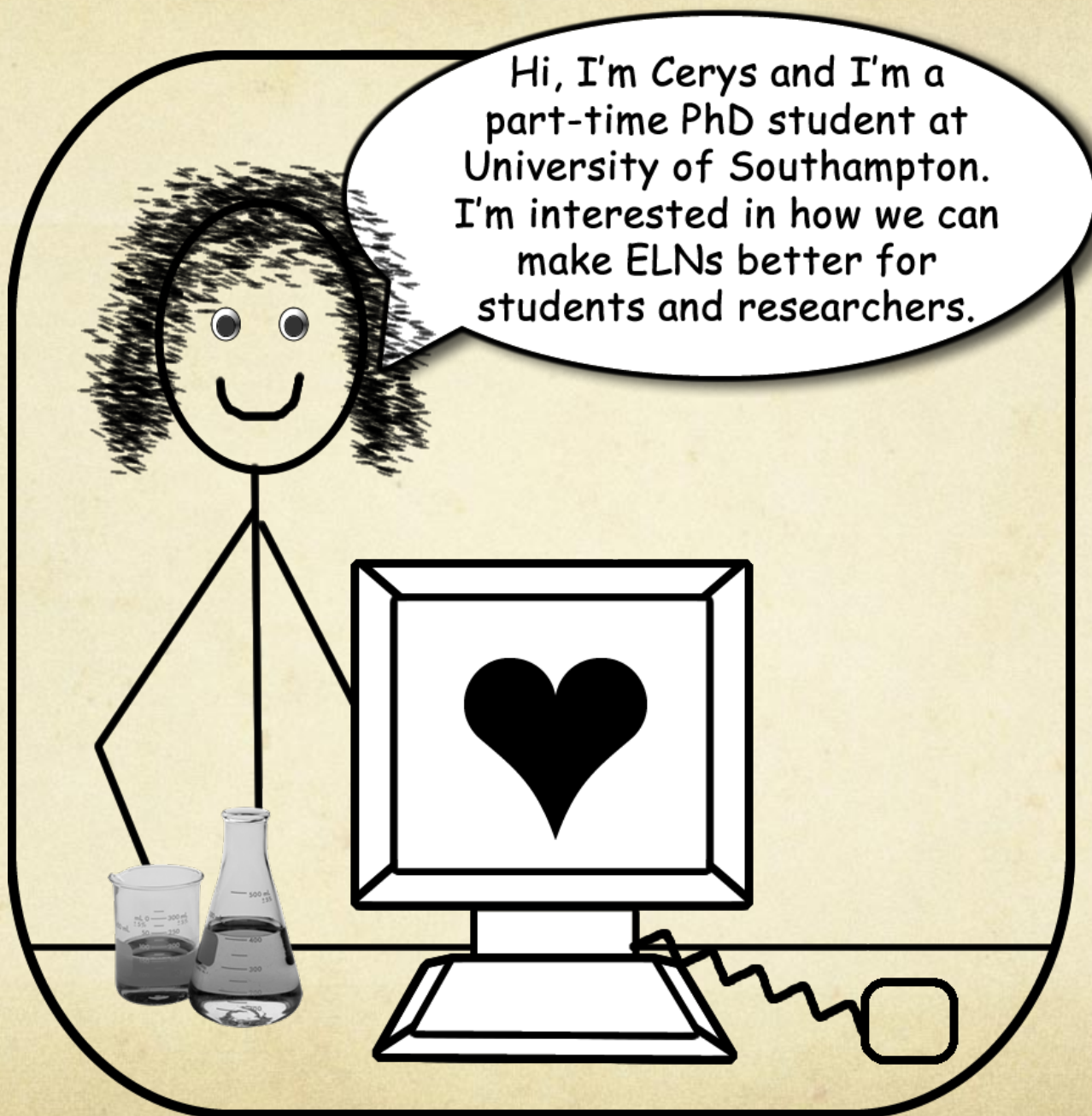


ELNs for researchers and students

A user perspective on ELNs in academic environments



LabTrove

“preserving the record”

© flickr.com/julia_manzerova

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our experiment

Pictet-Spengler route to Praziquantel


Success of intermediates and derivatives of PZQ

Order Posts: 1/1

Continuation: Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MWS6-9 to MWS6-12)
17th March 2013 10:07:29

Acid-catalyzed Pictet-Spengler using methanesulfonic acid in various concentrations

Continuation of Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MWS6-5 to MWS6-8)



MeSO₃H
various conditions

LabTrove enables the formation of a Smart Research

LabTrove
labtrove

labtrove Public Blog Post: Synthesis of amine-linked analogue of TCMDC-123812 via reductive amination...
<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/XhgyRb8i> #malaria #drugdesign
yesterday · reply · retweet · favorite

labtrove Public Blog Post: Synthesis of 2-Ethoxycarbonylthiolan-3-one
<http://t.co/m9mUBQKS> #malaria

<http://www.labtrove.org>

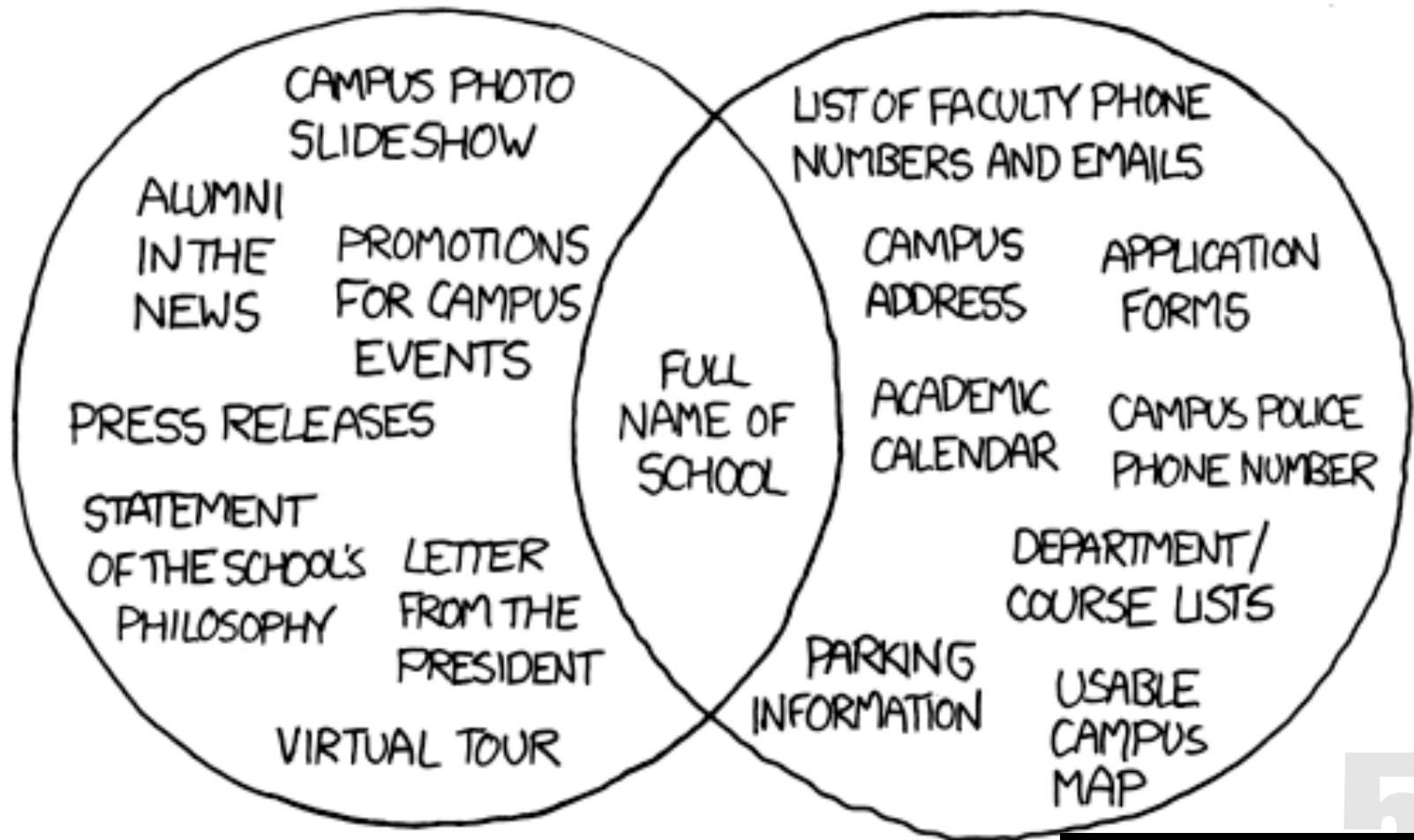
3

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

THINGS ON THE FRONT PAGE
OF A UNIVERSITY WEBSITE

THINGS PEOPLE GO TO
THE SITE LOOKING FOR





And making things
easy to use!

Different users have different needs



Undergraduates



Researchers



Supervisors

Who else might have needs?



Project
funders

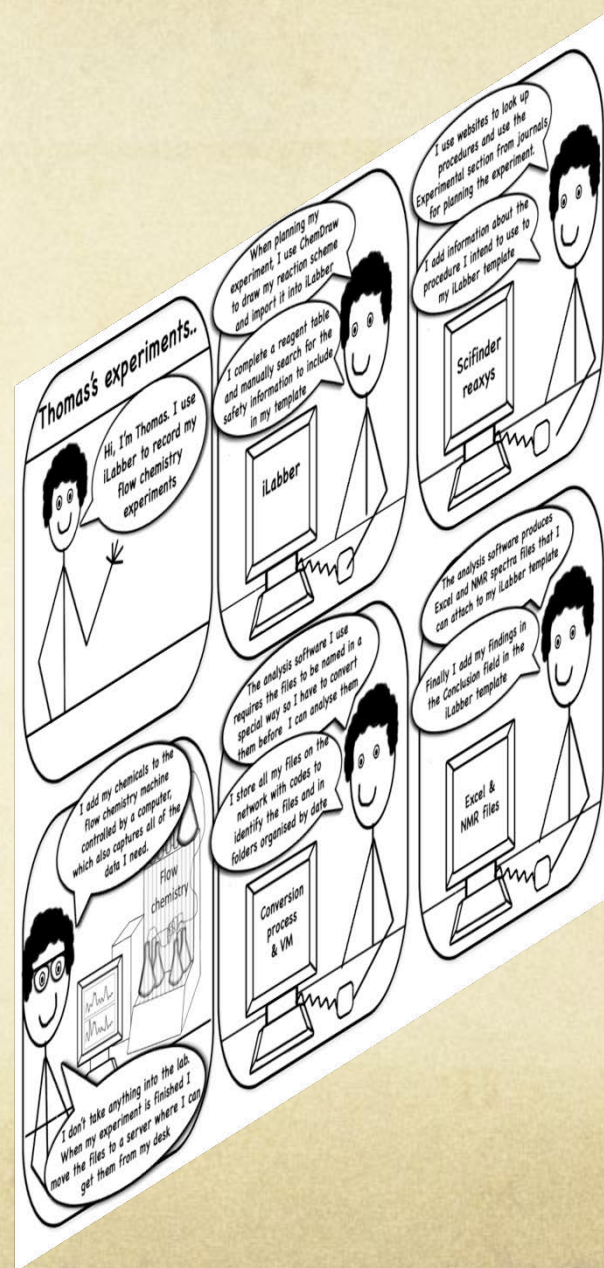
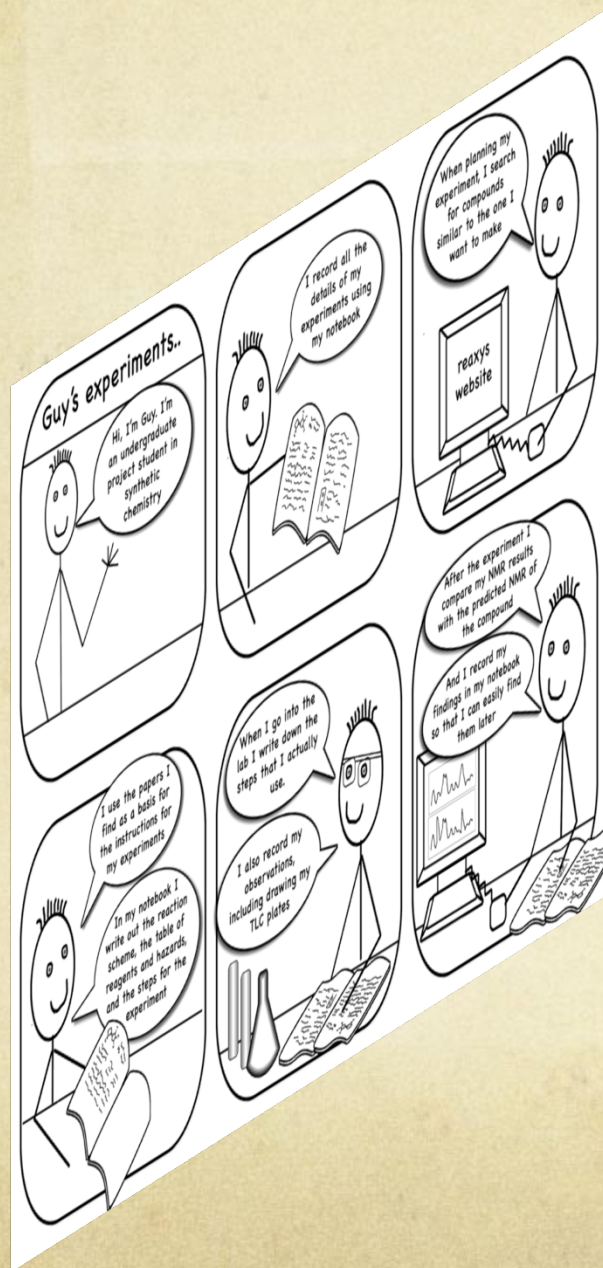


Collaborators



Future
students

Different ways of organising experimental information



Benefits to using ELNs in academic institutions

What matters to users?

A stack of light brown file folders is positioned in the upper left corner. The top folder has the word "CONFIDENTIAL" printed in bold, black, sans-serif capital letters. The background is a textured, aged, light beige paper with numerous black ink splatters and dots, particularly concentrated on the right side.

CONFIDENTIAL

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.**

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: OCtrl/ 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

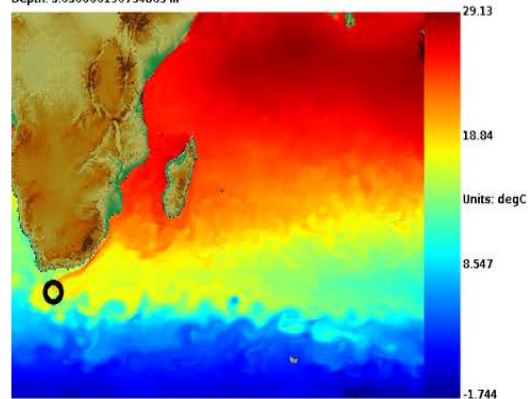
Elevationunits: m

Elevationpositive: down

Godiva2 test site for BlogMyData > HIGEM XBYLR Monthly means > OCtrl/ Temperature.

Time: 2010-08-16T00:00:00.000Z

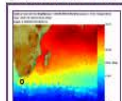
Depth: 5.050000190734863 m



Testing POI works

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.

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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

OCtrl/ Temperature. (6)

OCtrl/ Salinity. (2)

Density (5)

Calendarsystem

360 Day (13)

Elevationunits

M (13)

Elevationpositive

Down (13)

Tools

Show/Hide QR Code

Show/Hide Keys

BlogMyData Project - Godiva



Open access is controversial but has real benefits for some

3

Praziquantel – Open Science

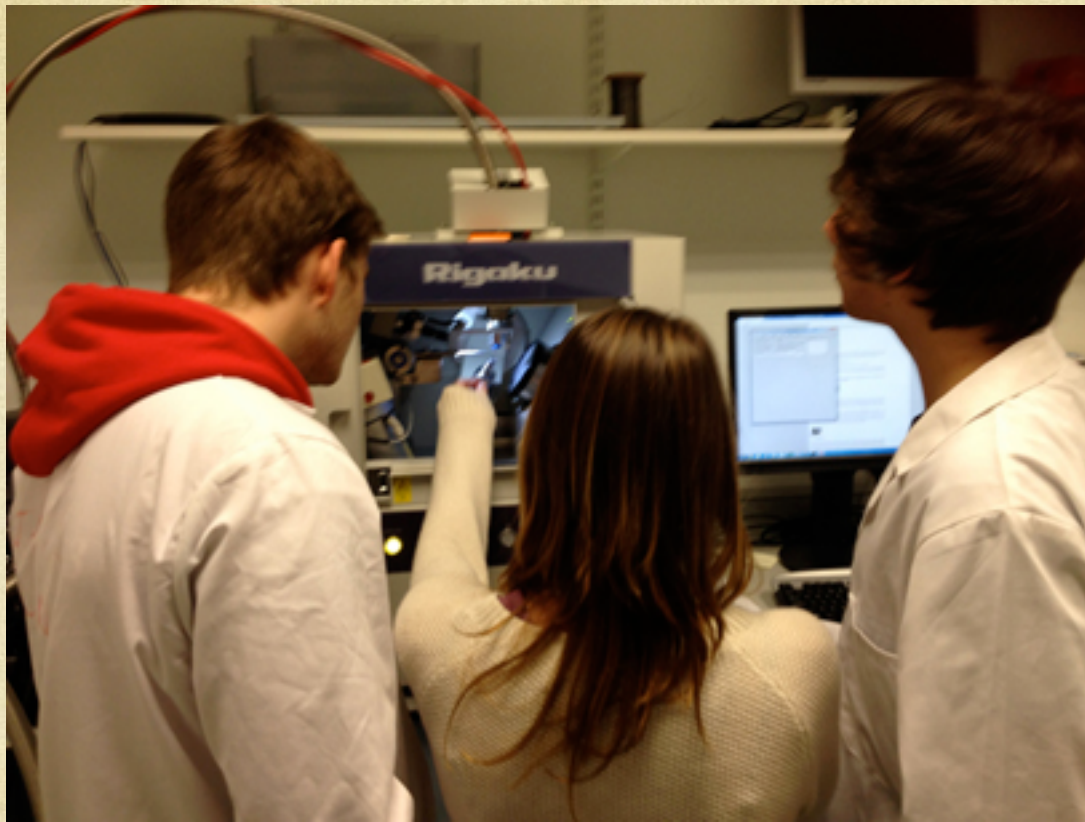
Pictet-Spengler route to Praziquantel

Racemization of PZQ and PZQamine

Racemic Resolution of Praziquantel and

Hydrolysis of PZQ

Introduction



Students

Training and standards



Typ Methyl ester Hydrolysis:- Method 2

9th April 2009 @ 16:50

Lab Note Book Or Experiment Code: FDH-5405-E7P26

Post Type: Method_2

Procedural Step: Method_2

Date Of Experiment: 27-11-08

Experiment Name: Typ_Methyl_ester_Hydrolysis

Experiment Code:FDH/5405/E7P26

Date of Experiment:27/11/08

- reaction mixture added to 100ml of DCM
- solid formed...dissolved in DCM/MeOH + water and evaporated to near dryness
- re dissolved in 200ml chloroform+20ml MeOH, sonicated most dissolved.
- 30ml water added myself leading to solid problems and poor separation seen.
- 100ml water added now gives clear layer with myself below
- transferred to bigger 500ml sep funnel.



this picture taken directly after transference

- approx. 30ml 2M hydrochloric added to give emulsion separation. and turn porphyrin protonated green.
- much better behavior now....lovely shade of green too.



protonated porphyrin with 2M HCl

- HCl reextracted with 100ml CHCl₃.
- fluffy brown noted between interface. contaminant?
- organic rinsed 5 times 100ml water. first rinse turns it back to purple



now purple organic with aqueous

- water re-extracted into chloroform 100ml and rinse 5 times H₂O.
- organic fractions combined and dried over anhydrous sodium sulfate



27-11-08 (2)

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

Experiment Name

[Preparation Of Fulleropyrrolidin](#)

[Alcohol:-Planning And Safety \(8\)](#)

[Preparation Of N-Glycine](#)

[\(amino-Ethoxy-Ethanol\) Tert](#)

[Butyl Acetate \(4\)](#)

[Preparation Of P-tert Butyl](#)

[\(bis\(cyanomethoxy\)dihydroxy}}](#)

[Calix \(2\)](#)

[Preparation 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 \(5\)](#)

[Preparation Of Fulleropyrrolidin](#)

[Alcohol \(repeat 2\) \(3\)](#)

[Preparation Of Fulleropyrrolidin](#)

[Alcohol \(repeat 2\) \(1\)](#)

[Typ 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](#)

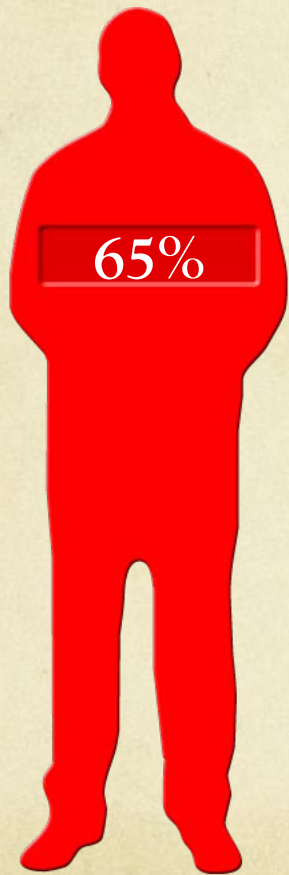
[\(1\)](#)

Support for students with disabilities

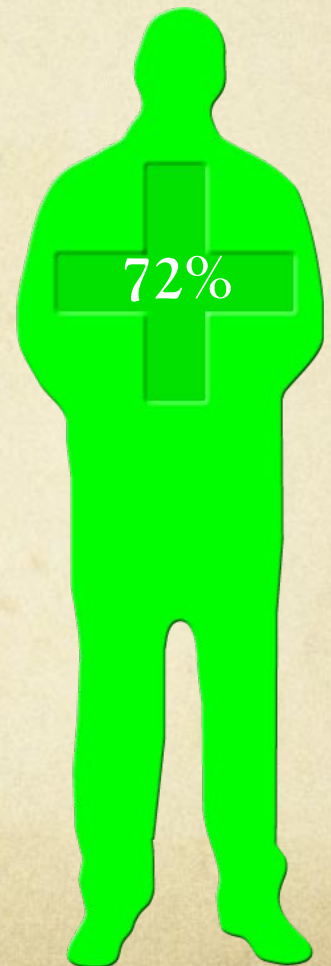


8

Undergraduate Advanced Crystallography Trial



Before



After

Attitudes towards ELNs

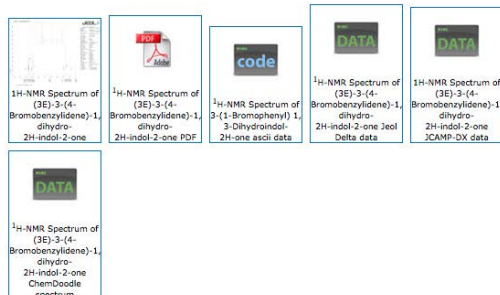


Data

Provenance & Citations

DOI's for Data

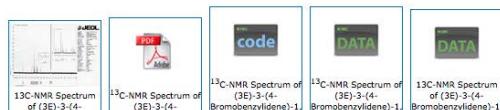
¹H-NMR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one
Spectroscopic Method: H-NMR
Substituent: Bromo
¹H-NMR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one



Interpretation of ¹H-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	vinyllic hydrogen on C ₈
8.28	broad singlet	n/a	1	amino hydrogen on N ₁

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



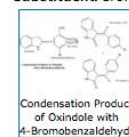
Reports

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

Graham Tizzari, Nicola Knight
 13th June 2013 | doi:10.5258/poc/lt/r/1

Condensation Product of Oxindole with 4-Bromobenzaldehyde

Substituent: Bromo

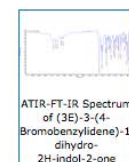


ATIR-FT-IR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

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 Number (cm ⁻¹)	Assignment	Remarks
3141	N-H stretching vibration (v(N-H) (1° amide))	Symmetrical stretching vibrations of the NH group
3077	Aromatic C-H stretching vibration (v(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

This Report

[Print view](#)

Availability

Currently:
Public (Googleable)

Make:

[Private \(Just For You\)](#)

[Notebook Users only](#)

Connecting physical & digital worlds

Room Blogs

Laser Environment

Environment

46:1047

21st July 2009

Auto blog

Data collected

46:1047

20th July 2009

Auto blog

Data collected

46:1047

19th July 2009

Auto blog

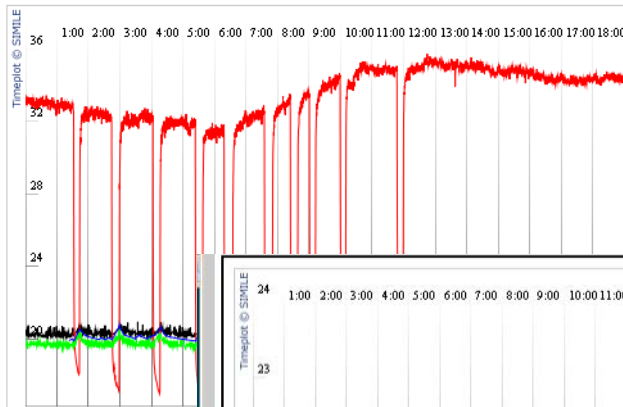
Data collected from 46:1047 on

[Auto Blogger](#) | [View](#)

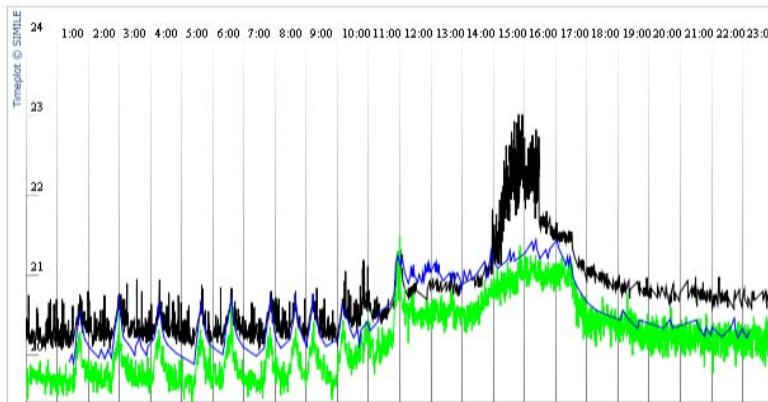
46:1047 - 2009-7-17

18th July 2009 @ 00:00

46:1047 - 2009-7-20



Chamber (46:1047/3/typeKthermocouple)
Plant Room (46:1047/0/typeKthermocouple)
Shelf top (46:1047/2/typeKthermocouple)
Laser box (46:1047/1/typeKthermocouple)



Chamber (46:1047/3/typeKthermocouple)	Black	<input checked="" type="checkbox"/>
Plant Room (46:1047/0/typeKthermocouple)	Red	<input type="checkbox"/>
Shelf top (46:1047/2/typeKthermocouple)	Green	<input checked="" type="checkbox"/>
Laser box (46:1047/1/typeKthermocouple)	Blue	<input checked="" type="checkbox"/>

Sortase Cloning - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://chemtools.chem.soton.ac.uk/p...

This is a repeat of the FP analysis from earlier in the... was run several times while the samples warmed up... seem to have settled down reasonably well

David Neylon | Proceed

Comments

Re: Repeat of FP analysis of Tus and GFP-Ter conjugate
3rd September 2007 @ 13:56

The data in the last few sheets will fit reasonably well to a simple binding isotherm. The actual values will not be terribly meaningful as there is an excess of unlabelled DNA in the reaction along with a significant amount of unlabelled GFP. This leads to the small change in FP.

Comment this post

Title:

Re: Repeat of FP analysis of Tus and GFP-Ter conjugate

http://chemtools.chem.soton.ac.uk - barcode_print.php (application/p...

Find



CODE: 4d4

Done

zotero

DNA_Conjugate (1)
Gel_electrophoresis (3)
DNA (2)
hybridisation (1)
protein_labelling (2)
Sample (1)
sample (19)
SDS_PAGE (1)
Fluorescence_analysis (3)

22

Automatic data from Matlab

blogs@xray

WSB Matlab Autoblog

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

Older Posts >>

This Blog

New Post

Timeline View

ion_vs_spot.m

14th May 2012 @ 11:59

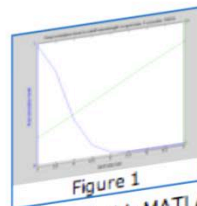
matlab code:

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



Published with MATLAB® 7.11.1

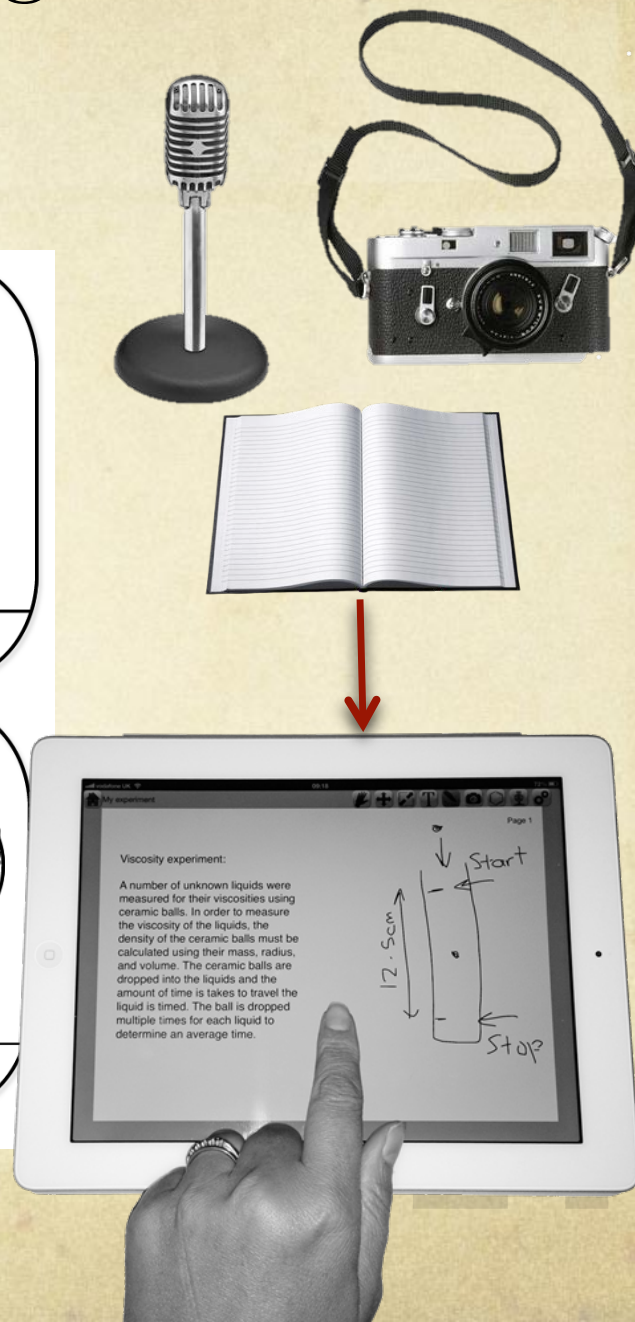
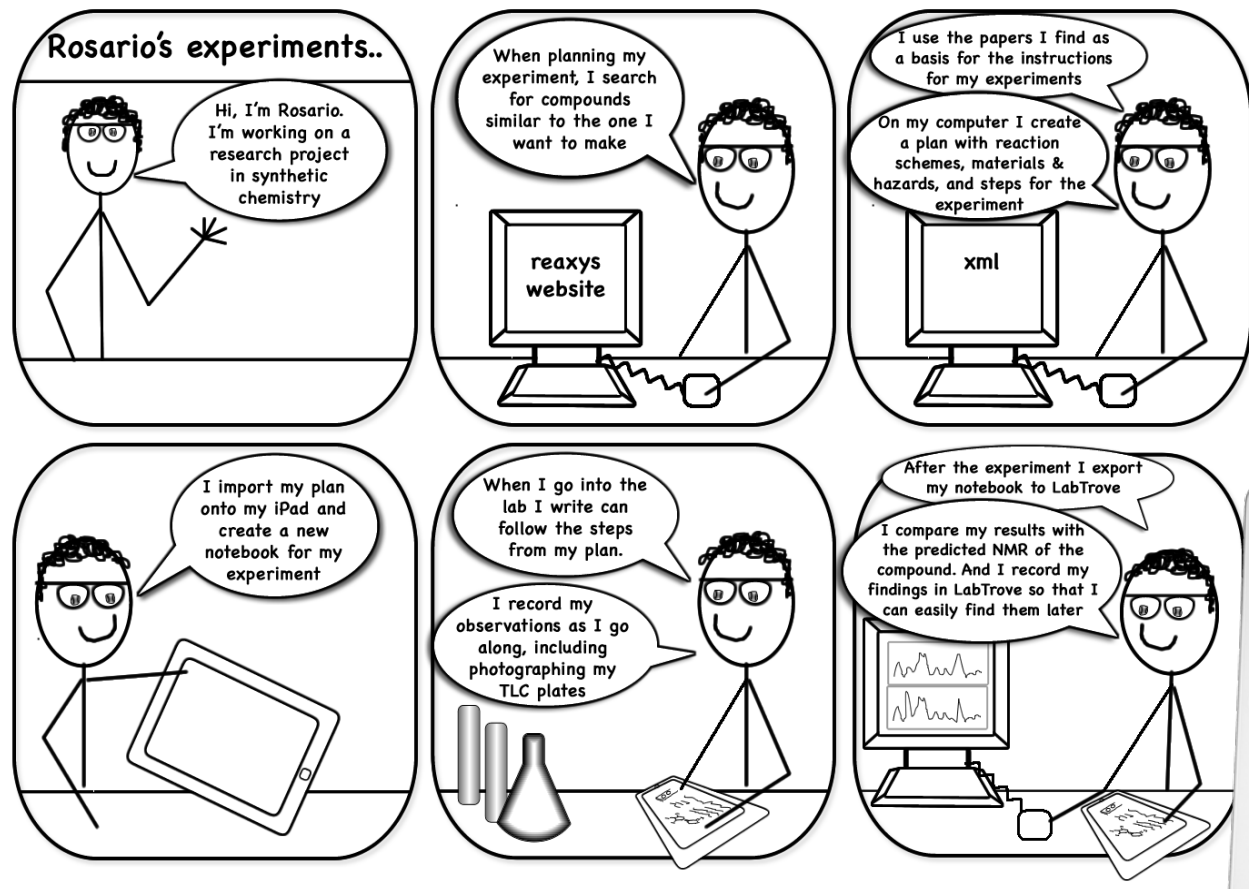
/Volumes/jfDfsResPhysicsAstronomyResearch\$/Private/xraylab/grants/2012 OPO HHG

Attached Files

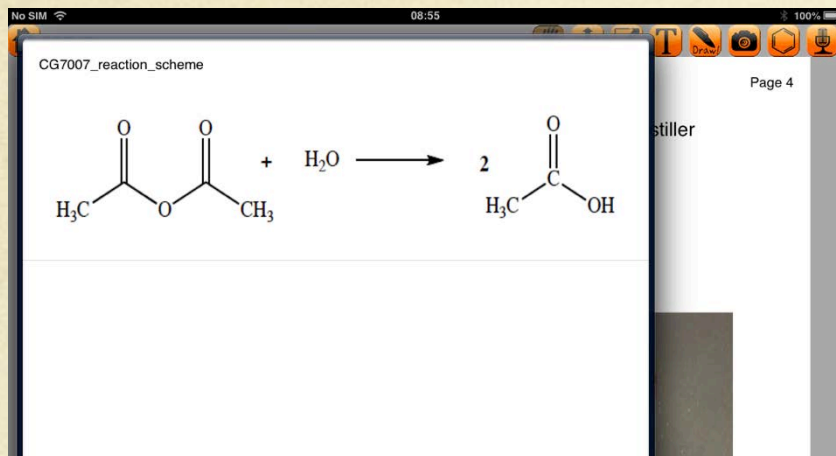
View Source | Matlab Autoblogging | Comments (0)

Computational processes can be run and captured

Flexible capture using mobile devices



Organic synthesis trial



mixing of 1-methyl-1H-pyrrole-2-carboxylic acid with thionyl chloride	Page 1
Heating to reflux	Page 3
Removal of thionyl chloride by vacuum transfert	Page 4
Dilution in diethyl ether	Page 5
addition of a 10 mL solution of Et3N with 2-bromoaniline	Page 6
Stirring for 6 h at room temperature	Page 7
Work-up of the solution (Quench with saturated NH4Cl, extraction with EtOAc, dried over MgSo4 and concentration under reduce...	Page 8

Page 4

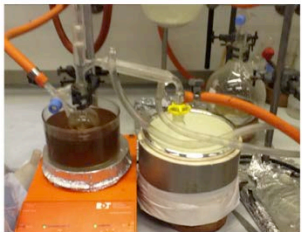
Name:	Moles:	Amount:	Safety:
1-methyl-1H-pyrrole-2-carboxylic acid	Planned: 0.00300 Actual: 0.00300	Planned: 0.38 g Actual: 0.38 g	GLP
2-bromoaniline	Planned: 0.00600 Actual: 0.00598	Planned: 1.03 g Actual: 1.03 g	Harmful if swallowed. Toxic in contact with skin. Causes damage to organs through prol...
triethyl amine	Planned: 0.00360 Actual: 0.00359	Planned: 0.50 mL Actual: 0.50 mL	— No smoking. Use personal protective equipment as required. IF IN EYES: Rinse ca...
thionyl chloride	Planned: 0.13785 Actual: 0.13785	Planned: 10.00 mL Actual: 10.00 mL	Harmful if swallowed Causes severe skin burns and eye damage Toxic if inhaled Do not...
diethyl ether	Planned: 0.14429 Actual: 0.19239	Planned: 15.00 mL Actual: 20.00 mL	— No smoking. Do not get in eyes, on skin, or on clothing.

Navigation: Last Step, List of Steps, Equipment, Reaction Scheme, Materials, + Add page, Next Step


CG7007

Step 3: Removal of thionyl chloride by vacuum transfert

Page 4



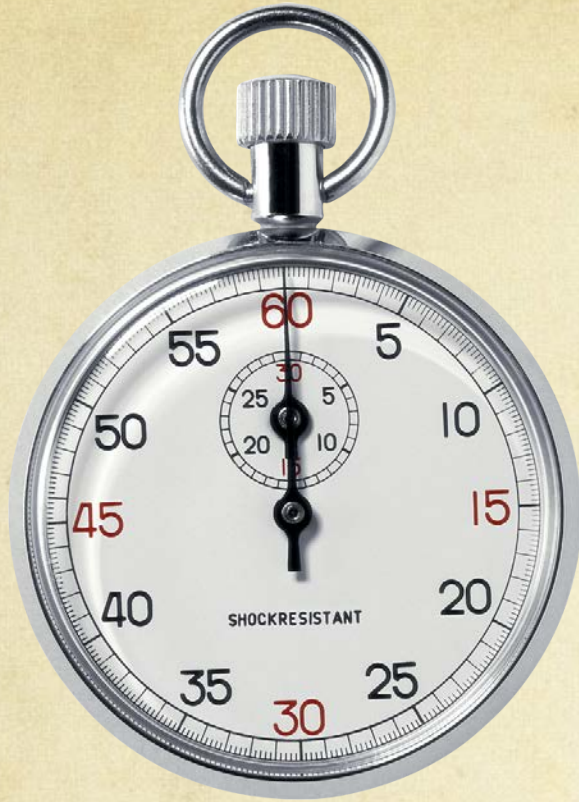
Rotavap vacuum was used. Distiller at room temperature



Crude visible as a brown oil.

No weighted, reaction continued to the next step with all the material

Navigation: Last Step, List of Steps, Equipment, Reaction Scheme, Materials, + Add page, Next Step



- 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?



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

“What I
Did”



90% used this
style with no
template

Do this



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

Further investigations..



With different templates and Lego!

materials

procedures

samples

Metadata

LabTrove and metadata

Automatic metadata
and
User-defined metadata

Section*

Analytical Procedures ▾

Metadata

key

value

Substituent

Nitro

Spectroscopic ▾

DSC

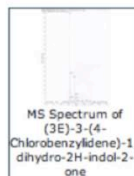
MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one

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:



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 mass and peak	molecular ions	Suspected molecules or ions	Inference
5=3			(M+H) ⁺ H(1)	Molecular ion gains a proton, ³⁷ Cl isotope present.
5=4			(M+He) ⁺ He(4)	Compound gains helium atom
5=33			(M+MeOH) ⁺ MeOH(32)	Molecular ion gains methanol, ¹³ C isotope present.
5=35			(M+H ₂ O+NH ₃) ⁺ H ₂ O(18), NH ₃ (17)	Molecular ion gains water and ammonia molecules
5=44			(M+CO ₂) ⁺ CO ₂ (44)	Compound gains carbon (IV) oxide molecule.
5=42			(M+Na+H ₂ O) ⁺ Na(23), H ₂ O(18)	Molecular ion gains water and sodium atom
5=18			(M+H ₂ O) ⁺	Compound gains water

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Tools

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Metadata Survey

blogs@ChemTools

The thoughts of Chemists

blogs@BioLab

Open output from the BioLab

ALTC Enotebook

our experiment
alpha



UNSW

THE UNIVERSITY OF NEW SOUTH WALES
SYDNEY • AUSTRALIA

enotebook

blogs@xray

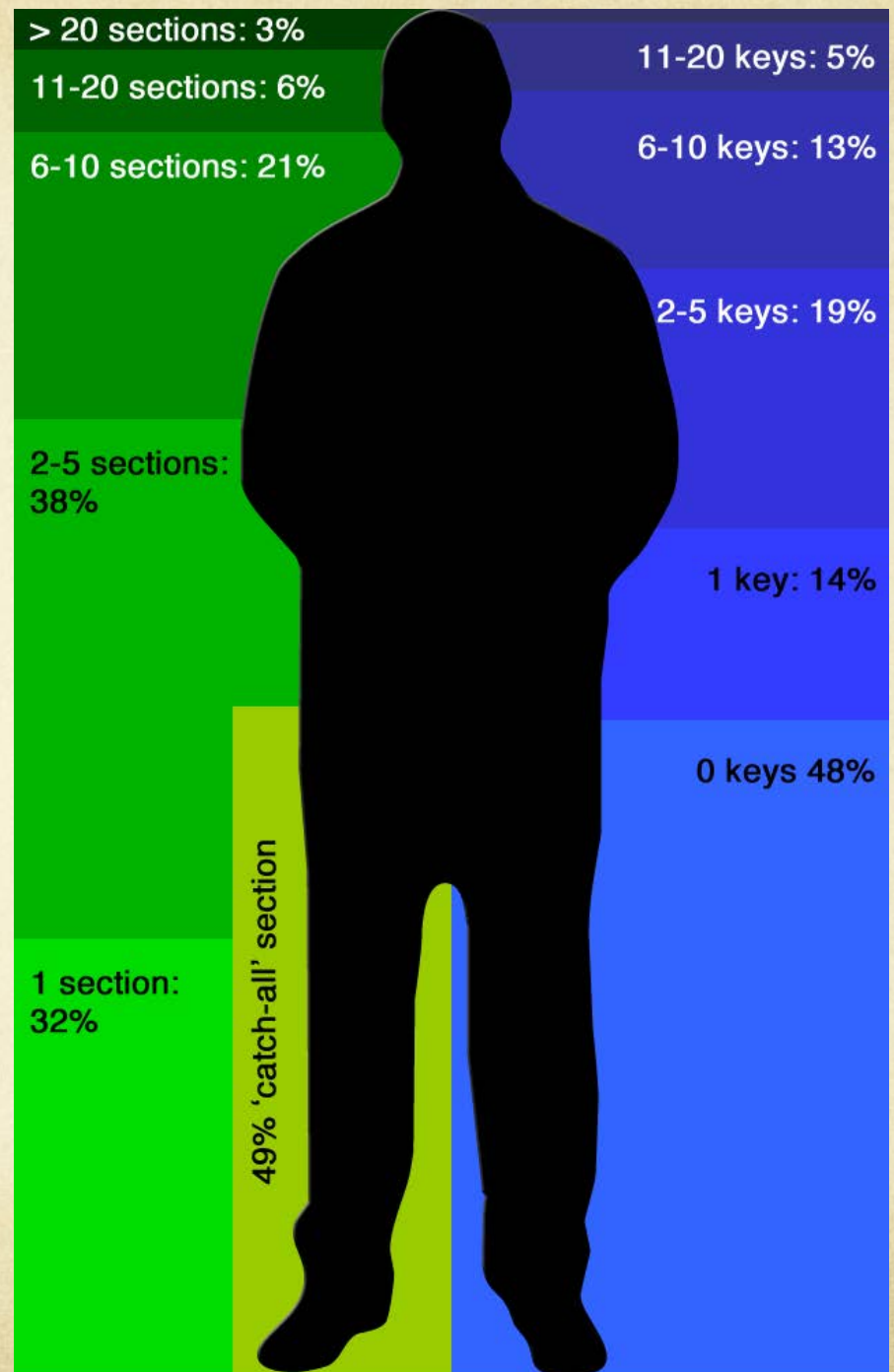
The thoughts of the ORC Xray Group

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..

A faint, multi-colored rainbow arc is visible in the background, spanning across the middle of the slide. The colors transition from red on the left to violet on the right, though the colors are somewhat muted and blend into the dark blue background.

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