

Generating metadata for an experiment: using a tablet ELN

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17th March 2014

LabTrove

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our experiment

Pictet-Spengler route to Praziquantel

Synthesis of intermediates and derivatives of PZQ

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Continuation: Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MW56-9 to MW56-12)
17th March 2011 @ 07:14

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

Continuation of Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MW56-5 to MW56-8)

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- March 2011 (3)
- February 2011 (3)
- August 2010 (3)
- July 2010 (3)
- June 2010 (14)
- May 2010 (3)

Sections

- Experiments (26)

Tools

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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/XhgyRb8i> #malaria #drugdesign
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labtrove Public Blog Post: Synthesis of 2-Ethoxycarbonylthiolan-3-one
<http://t.co/m9mUBQKS> #malaria

Metadata in LabTrove

Automatic capture of metadata

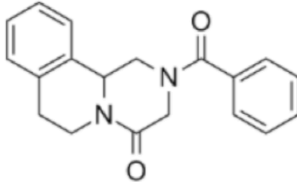


Enantioselective Hydrogenation of dehydro-PZQ and derivatives

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Preparation of MNR40-2

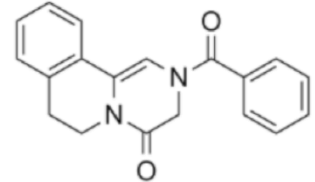
10th July 2012 @ 03:29



MNR14

→


sulphur
180 °C



MNR40

Compound	FW (g/mol)	mmol	Mass (g)	eq
MNR14	306.36	10.74	3.29	1.00
sulfur	32.07	21.48	0.69	2.00
MNR40-2	304.34			

Hazard and Risk Assessment:



HIRAC MNR37.pdf

Procedure:

A mixture of recovered SM from MNR40-1 (3.29 g, 10.74 mmol) and sulfur (0.69 g, 21.48 mmol) under argon was heated at 190°C in a sand bath for 2 hours.

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Metadata in LabTrove

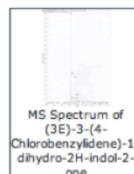
MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one

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	Suspected molecules or ions	Inference
258.2	258-255=3	(M+H) ⁺ H(1)	Molecular ion gains a proton, ³⁷ Cl isotope present.
259.2	259-255=4	(M+He) ⁺ He(4)	Compound gains helium atom
288.2	288-255=33	(M+MeOH) ⁺ MeOH(32)	Molecular ion gains methanol, ¹³ C isotope present.
		(M+H ₂ O+NH ₃) ⁺ H ₂ O(18), NH ₃ (17)	Molecular ion gains water and ammonia molecules
		(M+CO ₂) ⁺ CO ₂ (44)	Compound gains carbon (IV) oxide molecule.
		(M+Na+H ₂ O) ⁺ Na(23), H ₂ O(18)	Molecular ion gains water and sodium atom
		(M+H ₂ O) ⁺	Compound gains water

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URI Label
Revisions
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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

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Section*

Analytical Procedures

Metadata

key

value

Substituent

Nitro

Spectroscopic

DSC

Metadata Survey

UNIVERSITY OF
Southampton

blogs@ChemTools
The thoughts of Chemists

ALTC Enotebook



UNSW
THE UNIVERSITY OF NEW SOUTH WALES
SYDNEY • AUSTRALIA
enotebook

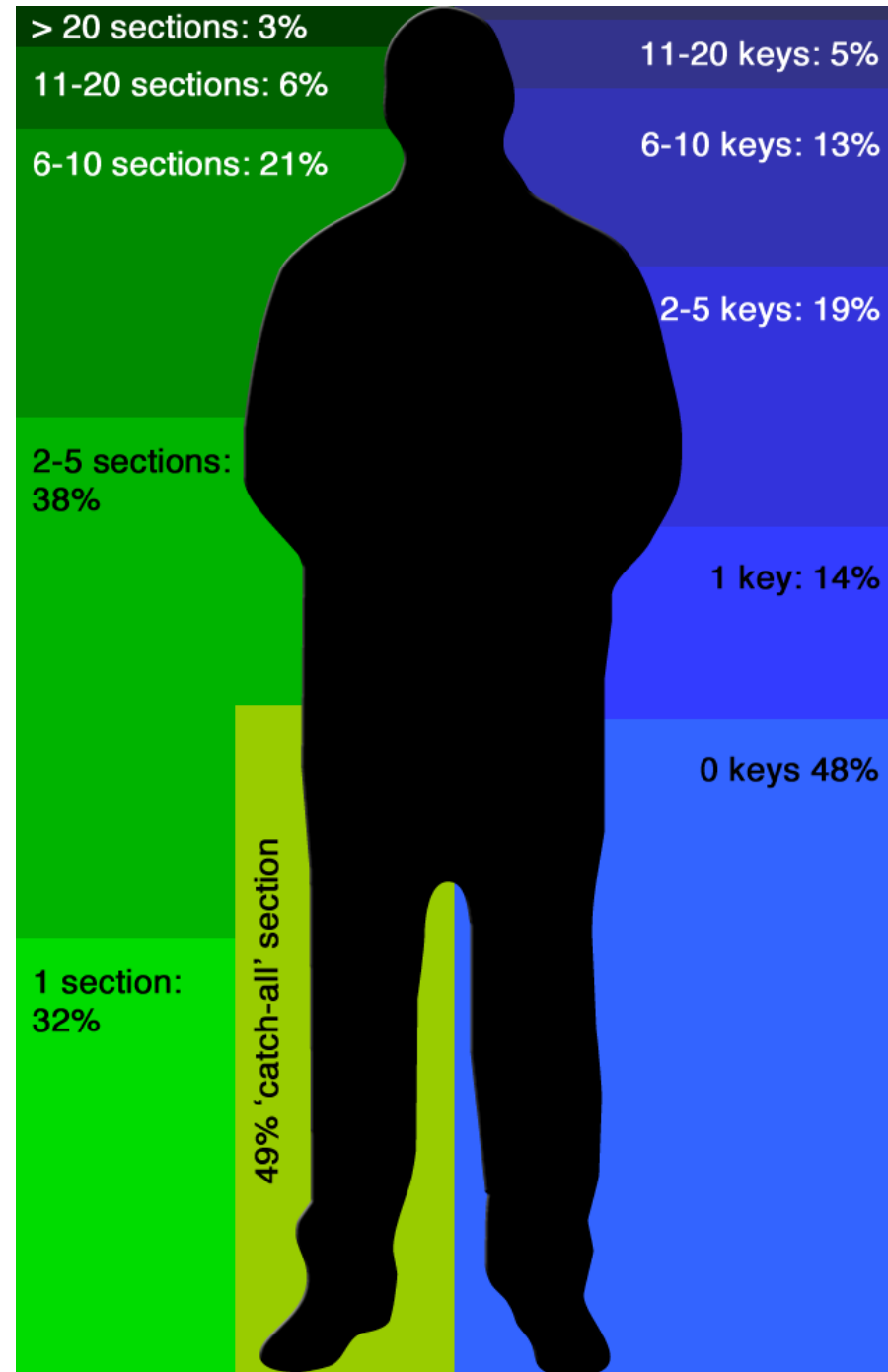
blogs@BioLab
Open output from the BioLab

our experiment
alpha

blogs@xray
The thoughts of the ORC Xray Group

104 blogs

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



Knowledge of how users already use metadata can help others

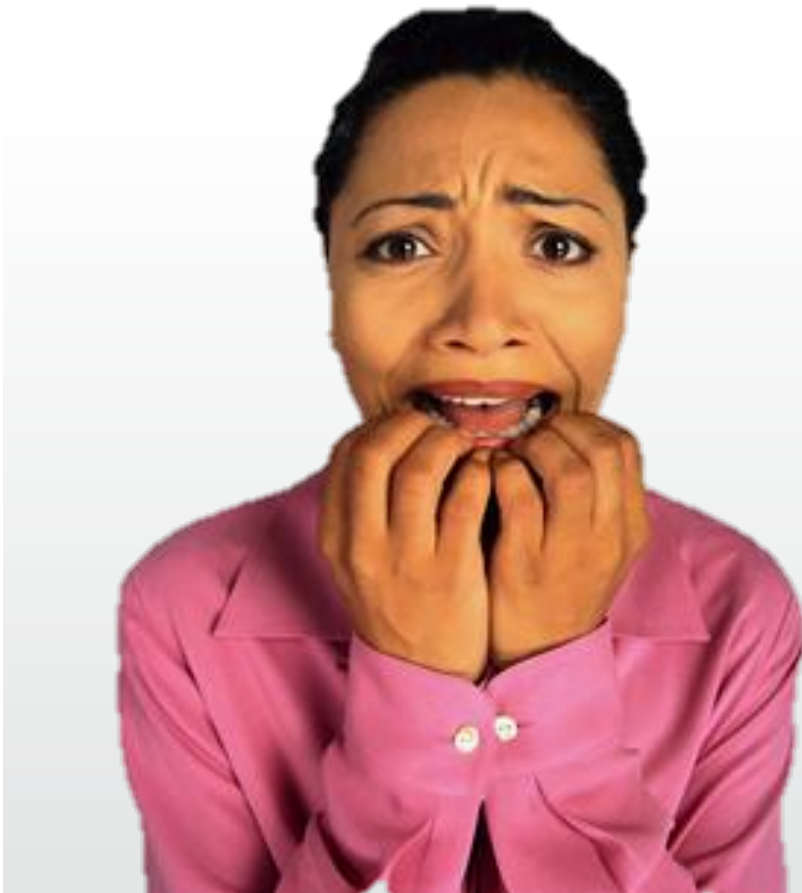


What do users do?

- User interviews
- User studies
- User observation

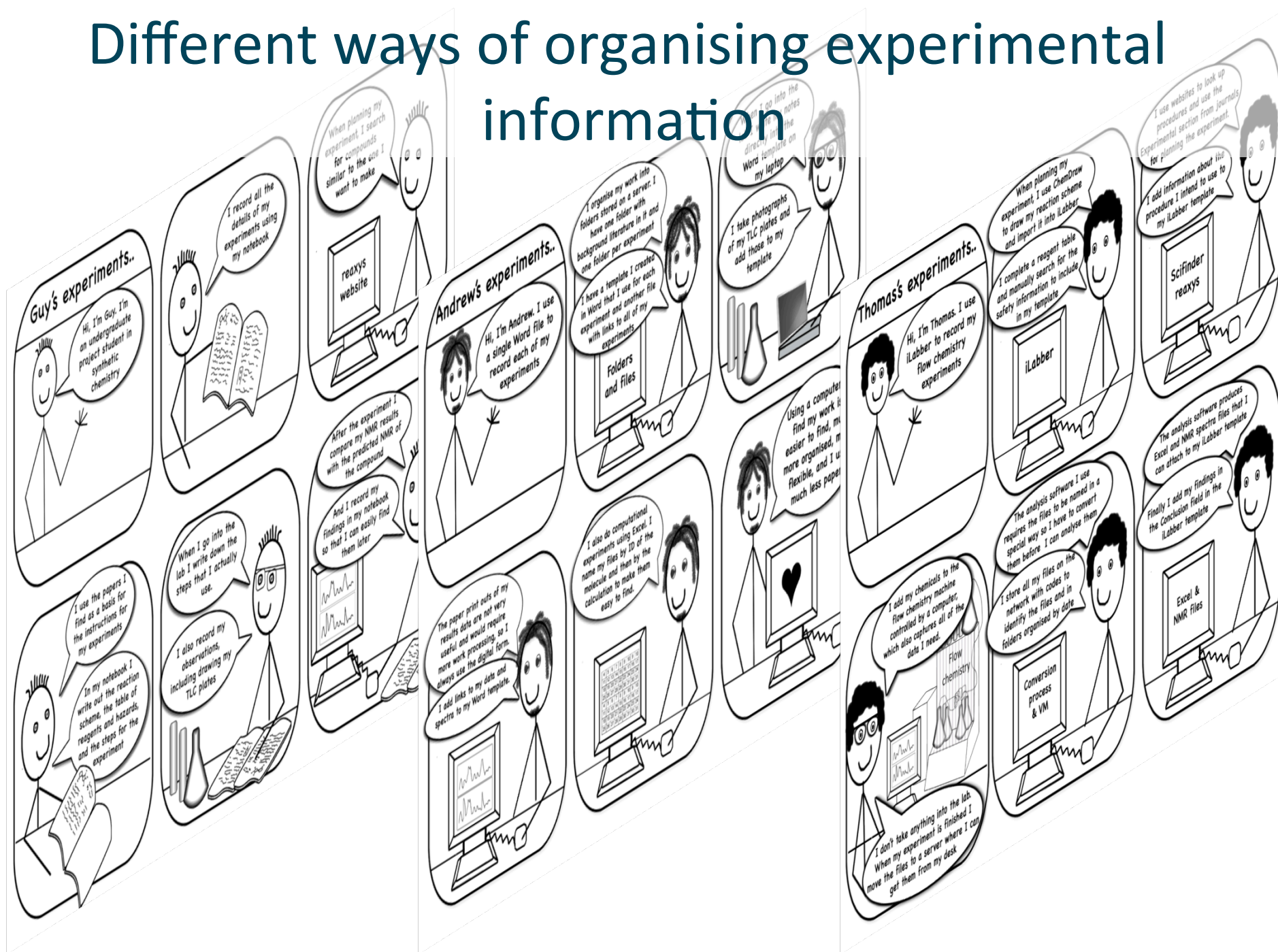


Metadata anxiety



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

Different ways of organising experimental information



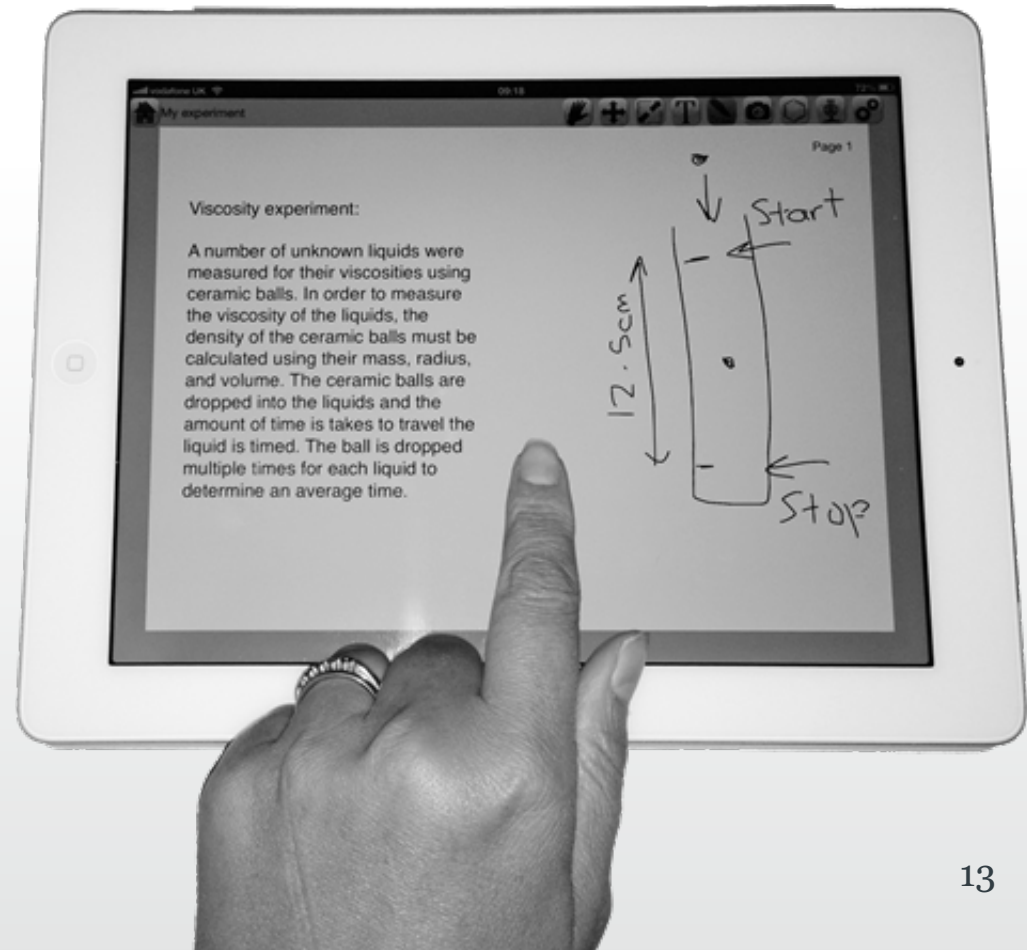
A background image of laboratory glassware, including a graduated cylinder and a round-bottom flask, with a blurred bookshelf in the background. The text is overlaid in the center.

We need to do more to
encourage effective
metadata capture

Developing a mobile ELN

- What is Notelus?





Providing guidance in an experiment

CG7007

Step 3: Removal of thionyl chloride

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

Crude visible

No weighted the next step

Last Step

List of Steps

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

Last Step

List of Steps

Equipment

Reaction Scheme

Materials

+ Add page

Next Step

- Experiment planning
- Describing the resources in the experiment

Also an opportunity to capture metadata



Metadata for every experiment

Configure the settings for your experiment

Project name:

Polymorphism advanced practical

Sub-project name:

Crystallisation

Conditions:

water

Description:

0.5g glycine in 20ml water. Heat to 60deg..... until dissolved. Crystallise by slow evaporation

Keywords:

glycine, polymorphism, crystallisation

Separate keywords using commas

Metadata derived from the plan

No SIM 08:55 100%

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.

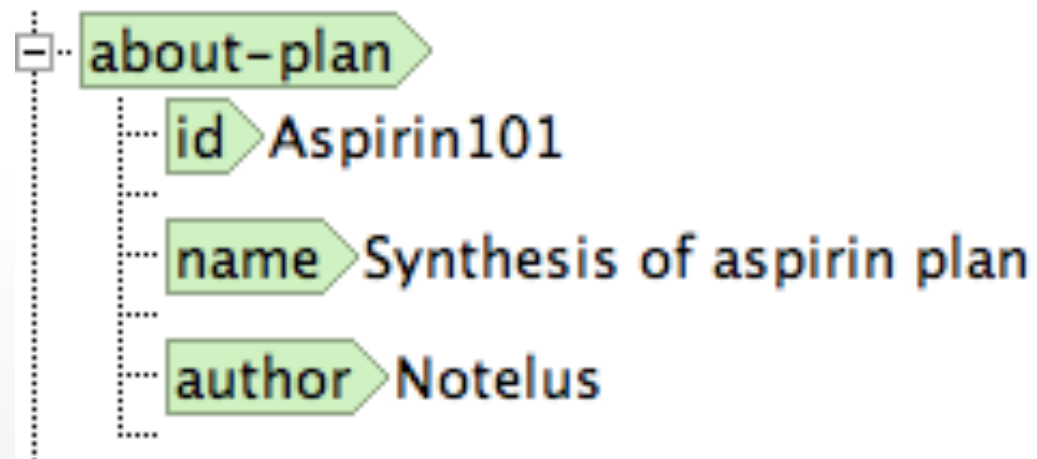
Page 4

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

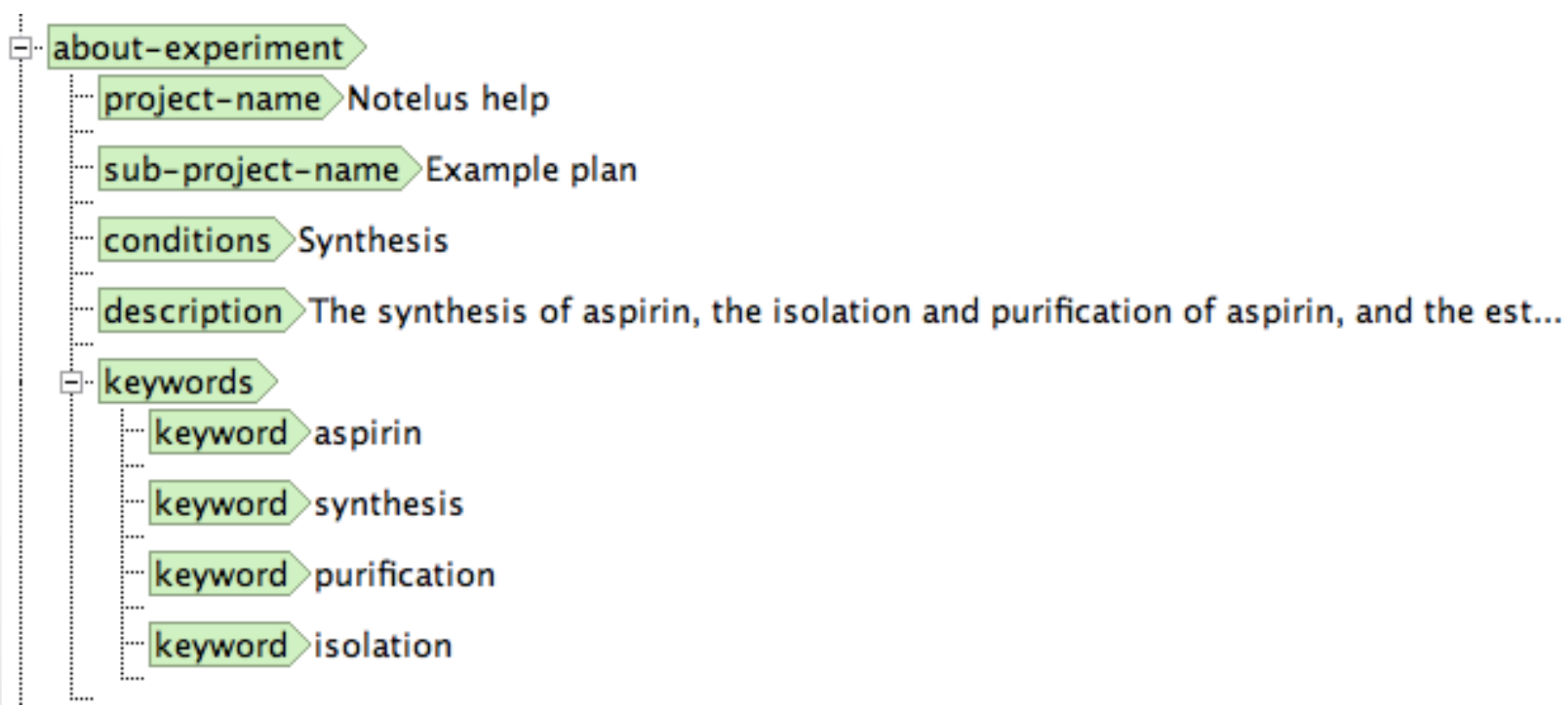
XML



Provenance for the plan



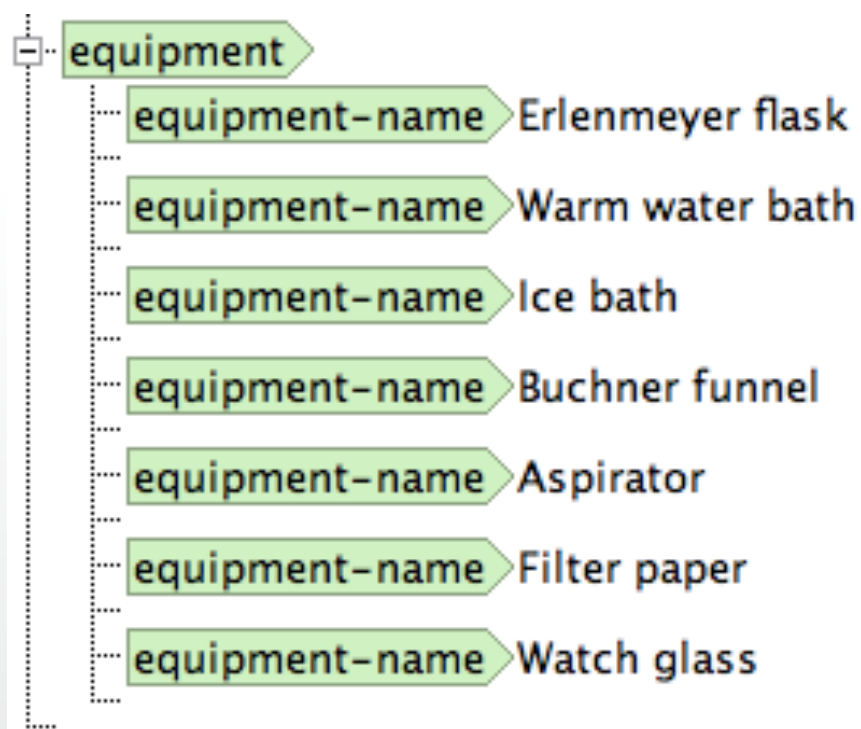
Pre-populating information about the experiment



Materials

-	material
	material-name Acetic Anhydride
	material-description Acetic anhydride, or ethanoic anhydride, is the chemical compound w
	material-safety Harmful on contact with skin – causes serious burns.
	molecular-weight 102.09
	density 1.08
	ratio 1
	planned-amount 3.50
	planned-amount-unit mL

Equipment



Getting the metadata into LabTrove

LabTrove Accounts

Post title: Experiment 1234D

Post content:

Experiment 1234D Proprties

Project name: Polymorphism advanced practical
Sub-project name: Crystallisation
Conditions: water
Description: 0.5g glycine in 20ml crystallised by slow evaporation
Keywords: glycine, ploymorphism, crystallisation

Include metadata: ☒ ON

Continue to posting options

Plan Id

01 (1)
Notebook From Plan (2)
Test02 (1)

Plan Author

Notelus (1)
Cerys (2)

Material

95% Ethanol (3)
Acetic Anhydride (3)
Acetylsalicylic Acid (3)
Concentrated H2SO4 (3)
Salicylic Acid (3)

Equipment

Kettle (3)
Mug (3)
Spoon (3)

Project

Polymorphism Practical (1)
Project Notelus (1)
Crystallography (1)
Viscosity (1)
Project X (2)

Sub-Project

Ceramic-ball Dropping (1)
Eclipse Sub Project (1)
Notelus-test-import-plan (1)
Crystallisation (1)

Conditions

Cool (1)
Nitrogen atmosphere (1)
Heated (1)
Evaporation (1)
Dilutions (2)
Viscosity, Time (1)

Keyword

crystallisation (2)
glycine (2)
polymorphism (2)
AB7 (2)
Topic 1 (1)
Topic 2 (1)
Topic 3 (1)
Y29 (1)

Plan Name

Vis01 (1)
Polymorphism Practical (1)

Futures

- This is just an example of what can be done
- Additional information could be captured
- Looking at alternative mark-up for plans and experiments
- Possible interface enhancements for LabTrove

- We can do more to encourage effective metadata capture in LabTrove as well



LabTrove – Aurora

CerysTest

What would you like to post?

Search 



Project



Background



Plan



Experiment



Data



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LabTrove – Aurora

CerysTest

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


Title*

Text*



Font Family

Font Size

B *I* U ABC \times \times^3         

Path: p



Summary



Materials



Instruments



Methods



Keywords



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Summary

Experiment reference

Project

Conditions

Add

high-pressure X

low-temperature X

nitrogen-atmosphere X

[Choose from your conditions](#)

Time period

From:

September



To:

October



☐ Experiment is complete

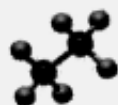
Description

Save

Cancel



Summary



Materials

What materials are you using in your experiment?

Add

triethyl amine X

2-bromoaniline X

1-methyl-1H-pyrrole-2-carboxylic acid X

diethyl ether X

thionyl chloride X

[Choose from your materials](#)

☐ Add recommended materials using ChemSpider



Instruments

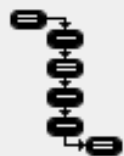
What instruments are you using in your experiment?

Add

Laser X

Electrospray X

[Choose from your instruments](#)



Methods



Keywords



Other



What type of information do you want to add to your experiment?

Location



Add values for this information

Add

B29:101 X

Laser-room X

Save

Cancel

Summary

- Challenges associated with metadata use
- Metadata can be usefully derived from a plan
- Providing interfaces to help
- We're looking at what else can be done ..

Metadata Study

<http://sites.google.com/site/cmetastudy/>



