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# Generating metadata for an experiment: using a tablet ELN

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17th March 2014

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# LabTrove


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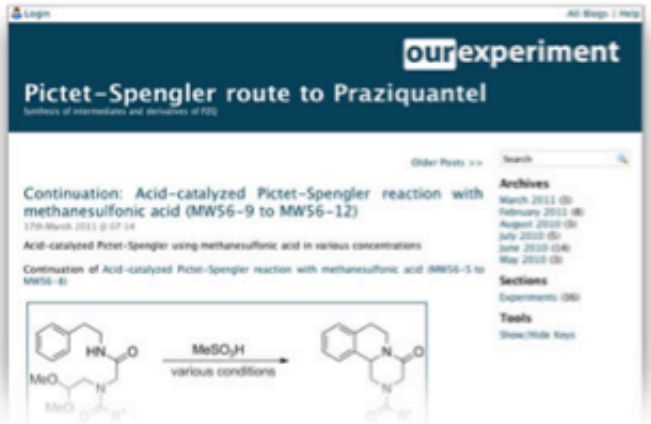


LabTrove enables the formation of a Smart Research

# Metadata in LabTrove

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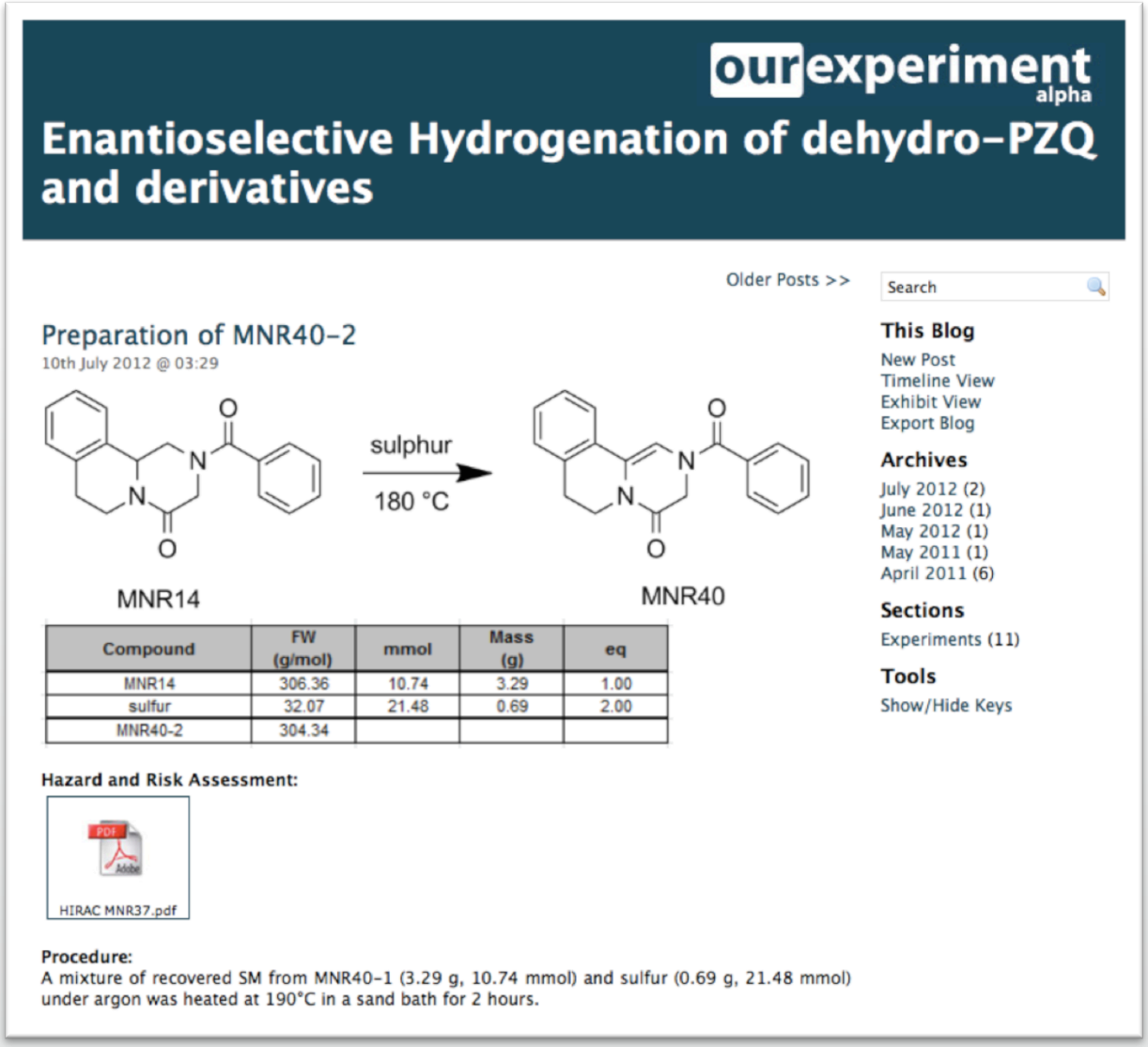
Automatic capture of metadata



ourexperiment alpha

## Enantioselective Hydrogenation of dehydro-PZQ and derivatives

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### Preparation of MNR40-2

10th July 2012 @ 03:29




MNR14 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

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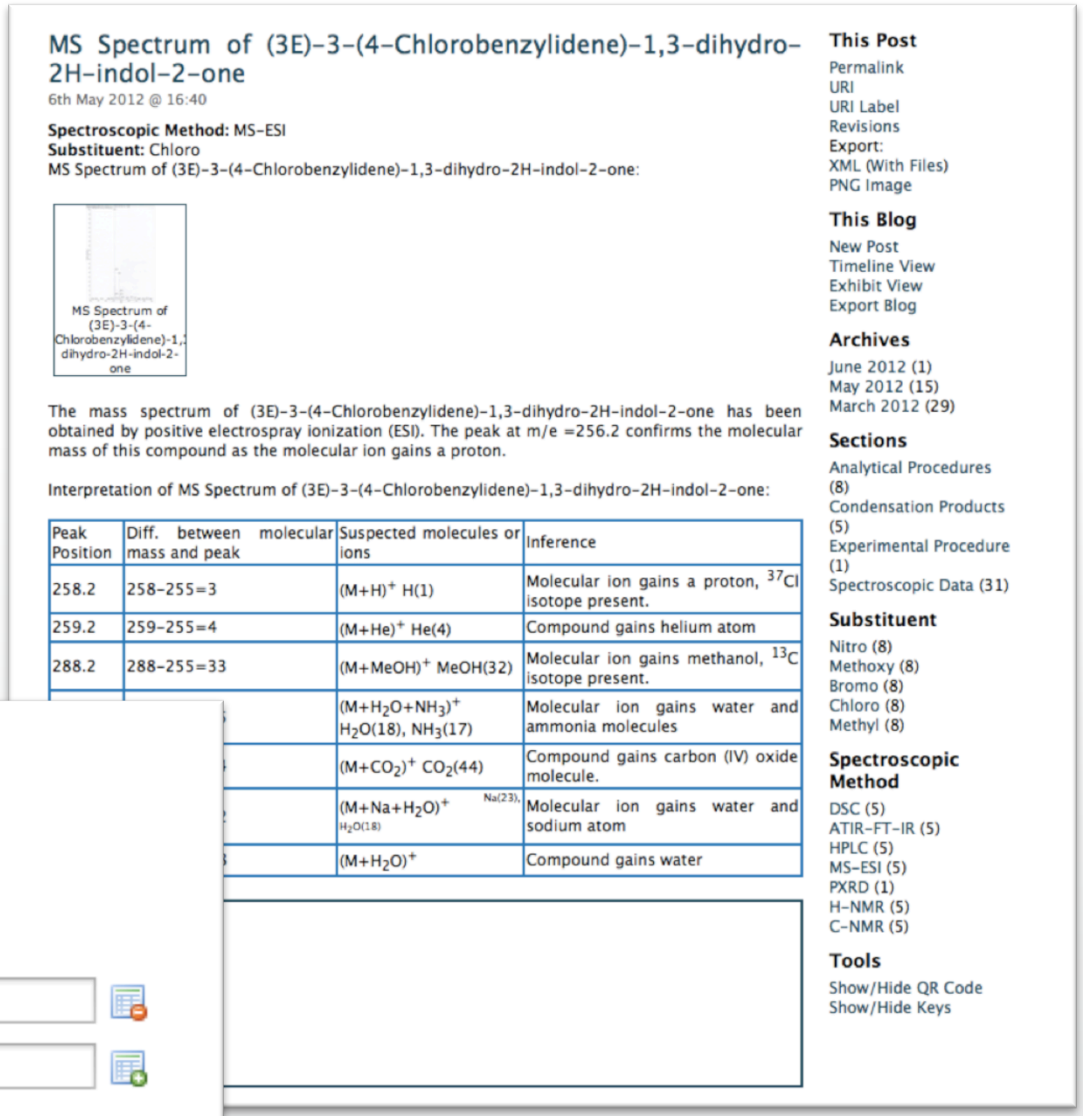

MS Spectrum of (3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one

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 |
|---|---|---|---|
| 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. |
| | | $(M+H_2O+NH_3)^+$ $H_2O(18)$, $NH_3(17)$ | Molecular ion gains water and ammonia molecules |
| | | $(M+CO_2)^+$ $CO_2(44)$ | Compound gains carbon (IV) oxide molecule. |
| | | $(M+Na+H_2O)^+$ $Na(23)$, $H_2O(18)$ | Molecular ion gains water and sodium atom |
| | | $(M+H_2O)^+$ | Compound gains water |

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Permalink
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Export Blog

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June 2012 (1)
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**Sections**
Analytical Procedures (8)
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**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

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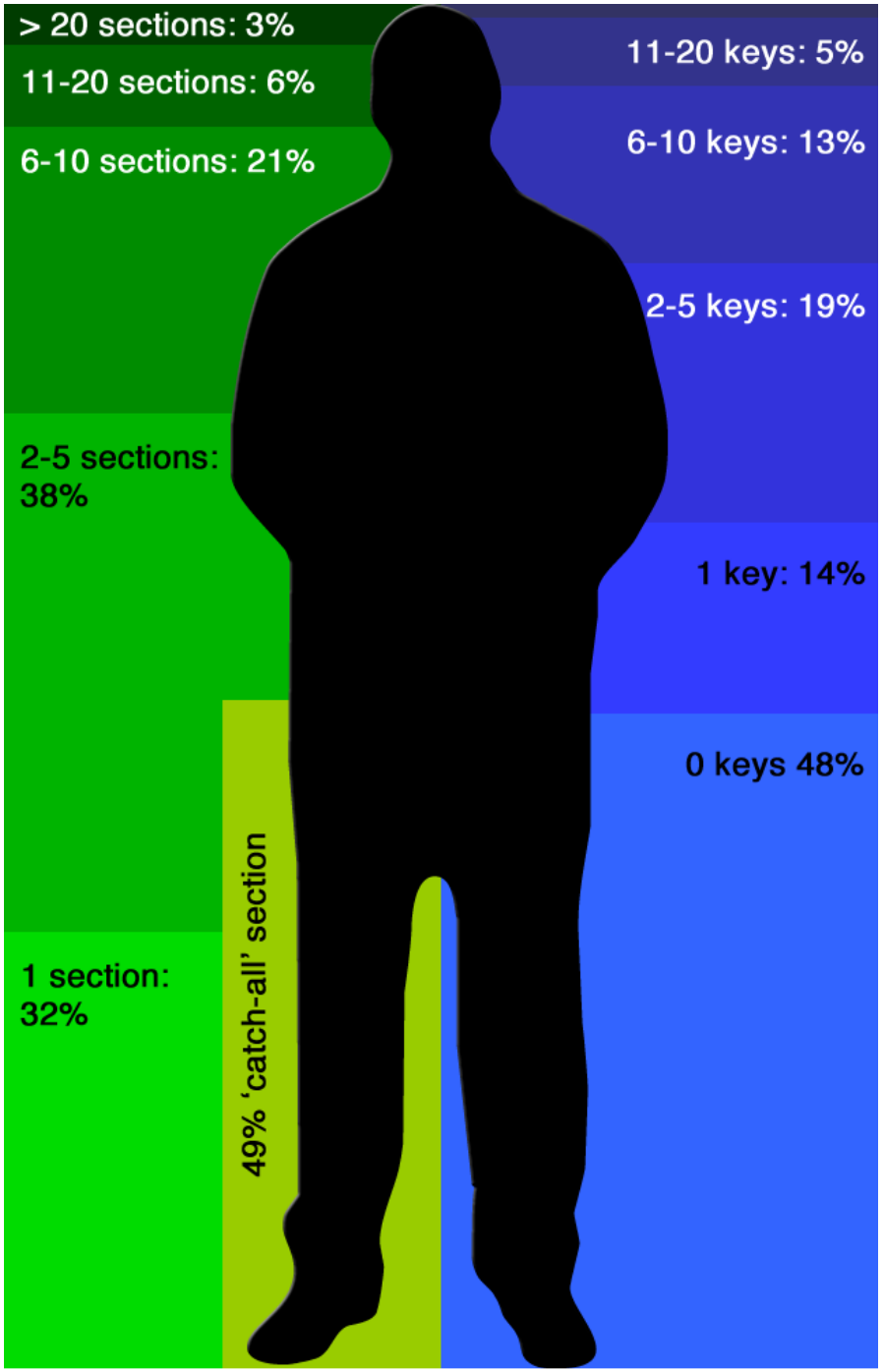
104 blogs

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



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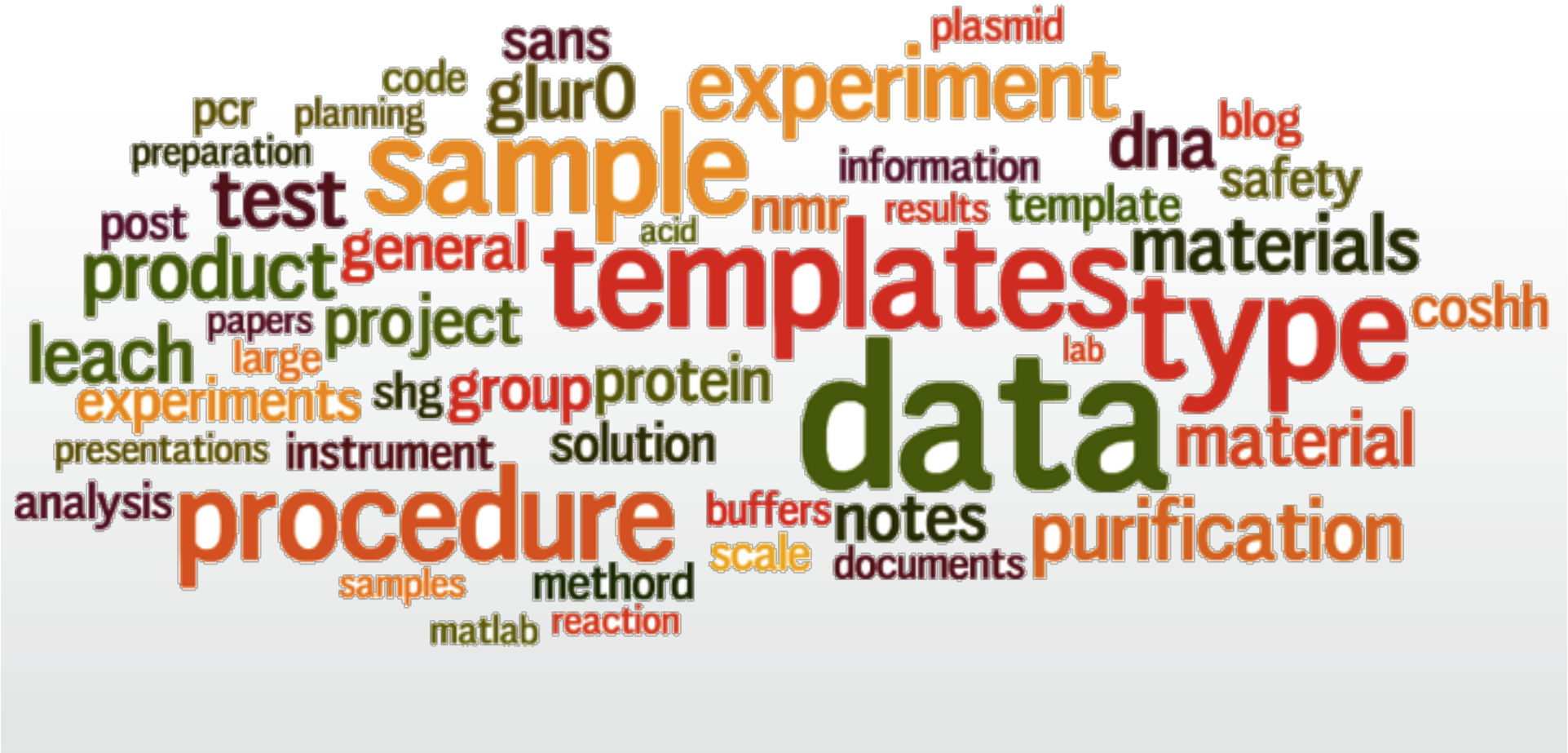
# Knowledge of how users already use metadata can help others



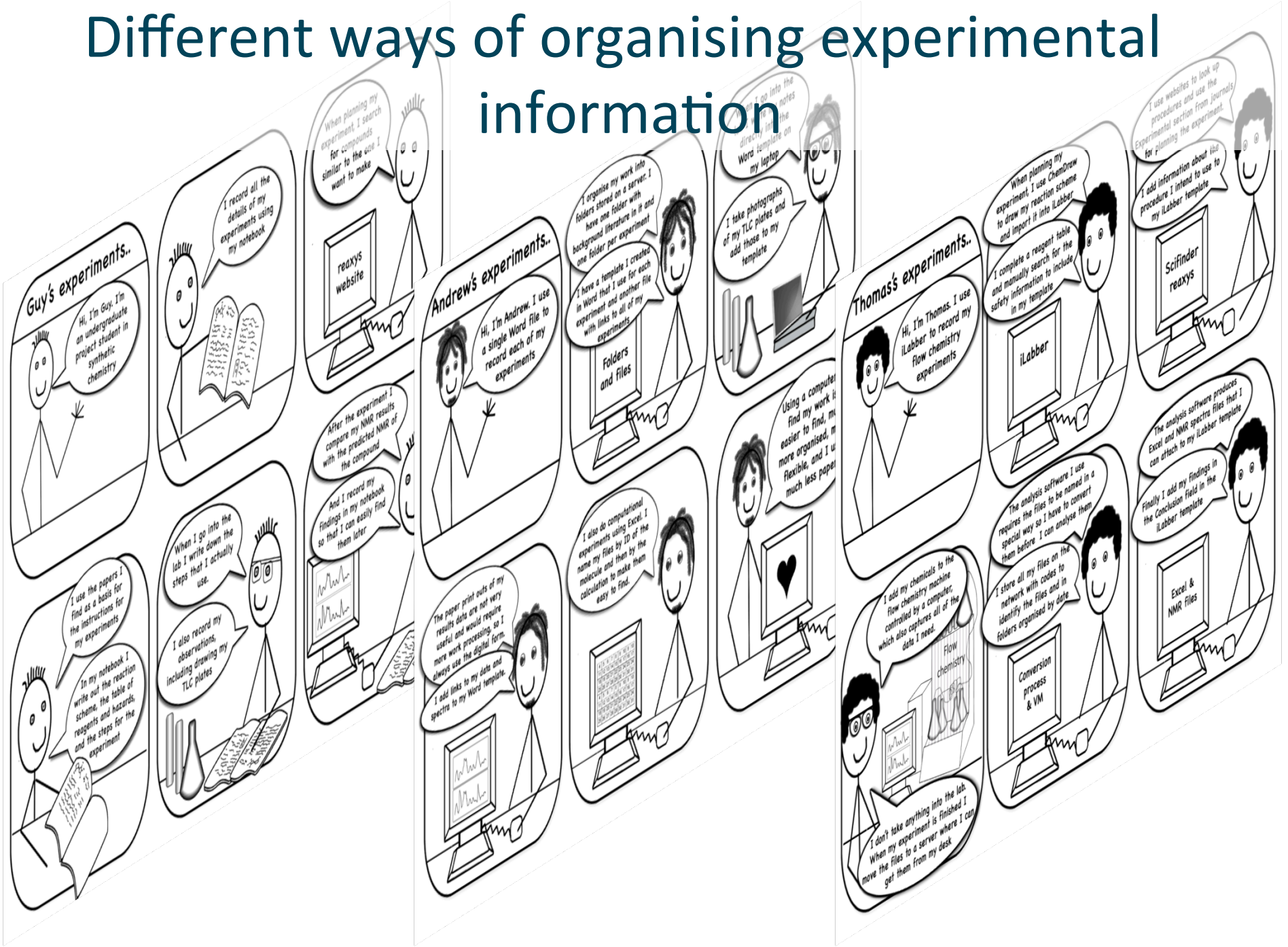
# What do users do?

- User interviews
- User studies
- User observation

# Metadata anxiety

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

# Different ways of organising experimental information




We need to do more to encourage effective metadata capture

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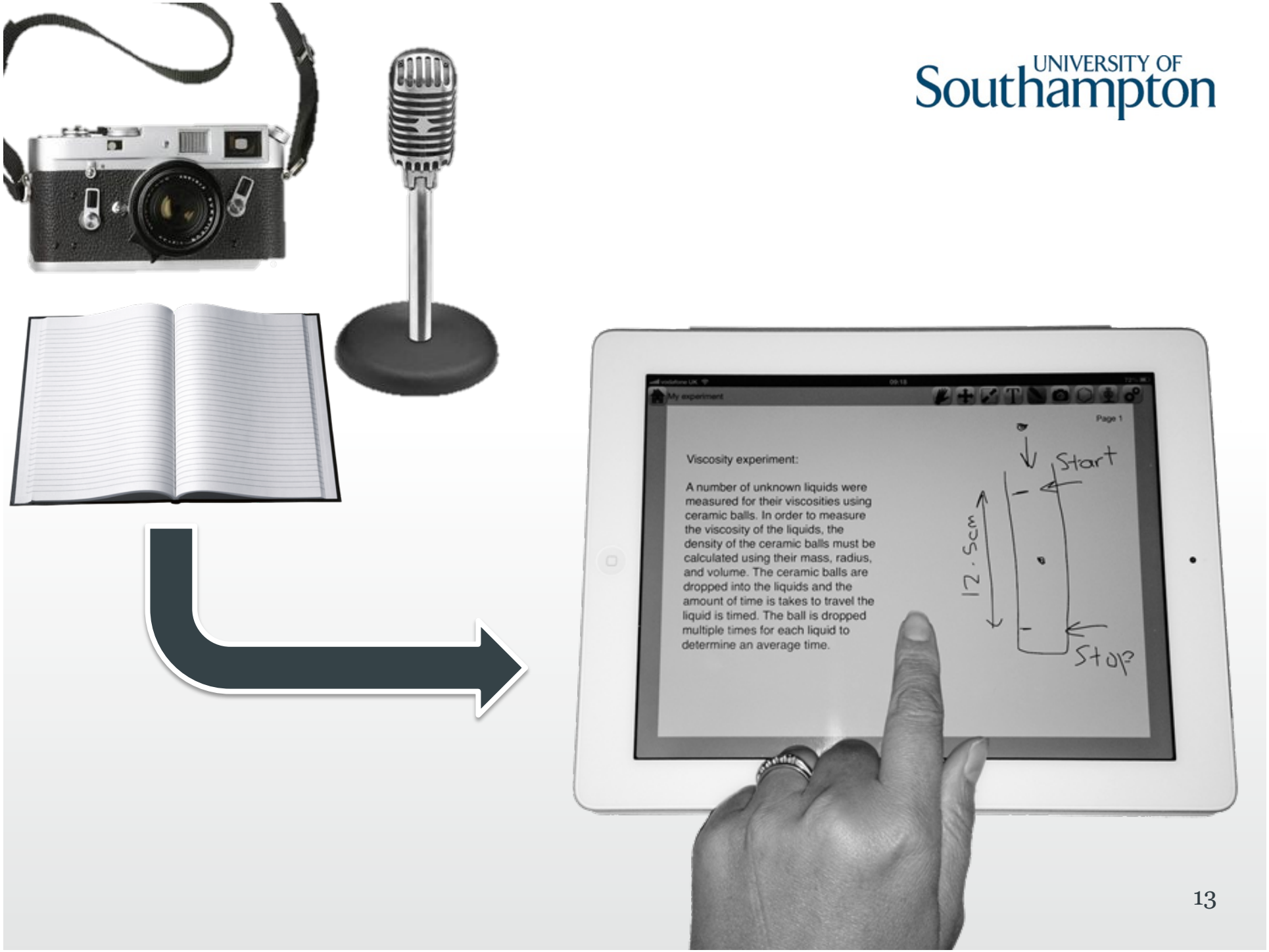
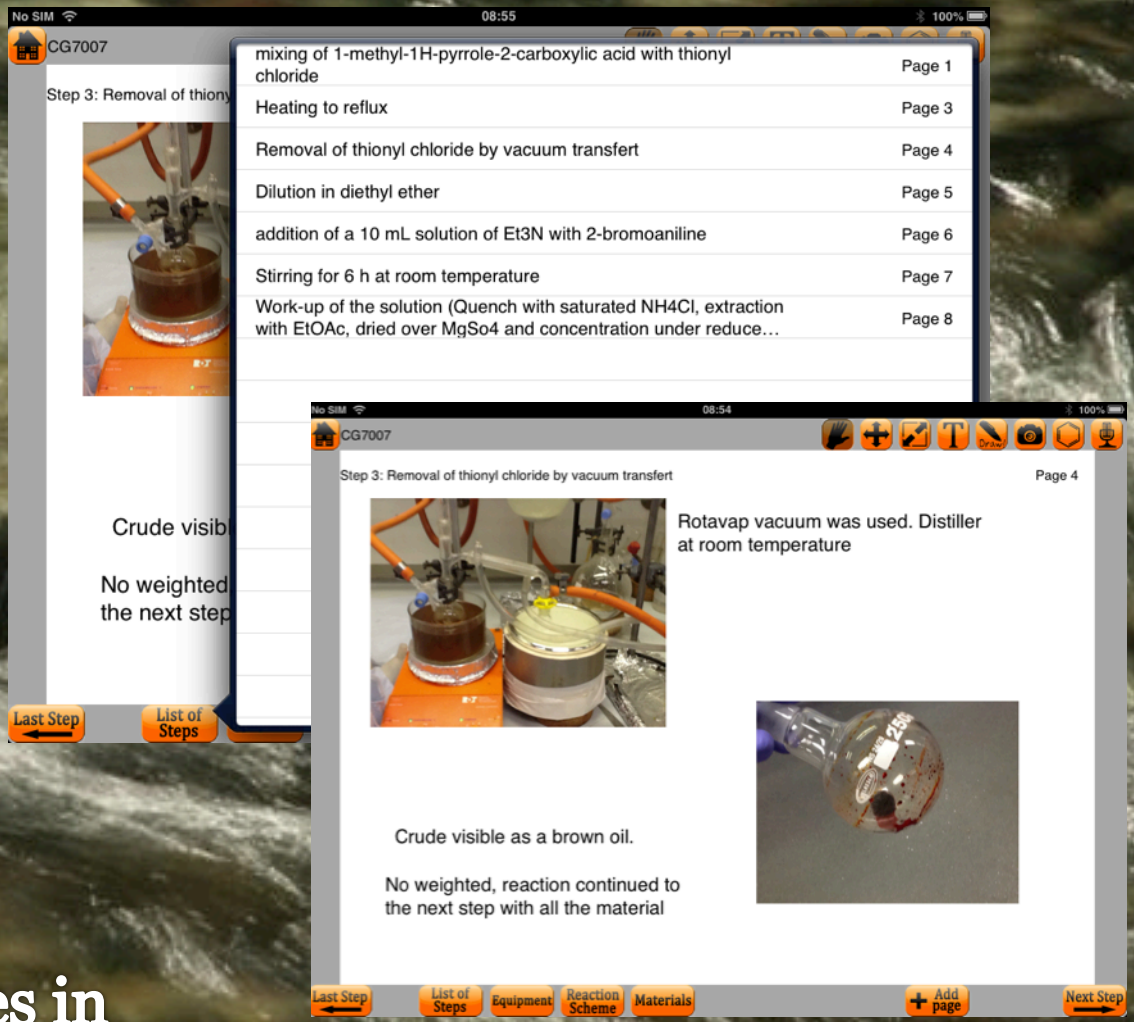
# Developing a mobile ELN

- What is Notelus?


My experiment
Page 1
Viscosity experiment:
A number of unknown liquids were measured for their viscosities using ceramic balls. In order to measure the viscosity of the liquids, the density of the ceramic balls must be calculated using their mass, radius, and volume. The ceramic balls are dropped into the liquids and the amount of time is takes to travel the liquid is timed. The ball is dropped multiple times for each liquid to determine an average time.
Start
12.5cm
Stop

# Providing guidance in an experiment




- Experiment planning
- Describing the resources in the experiment

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# Also an opportunity to capture metadata

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# 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 60degs until dissolved. Crystallise by slow evaporation |
| Keywords: | glycine, polymorphism, crystallisation |

Separate keywords using commas

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# Metadata derived from the plan


XML

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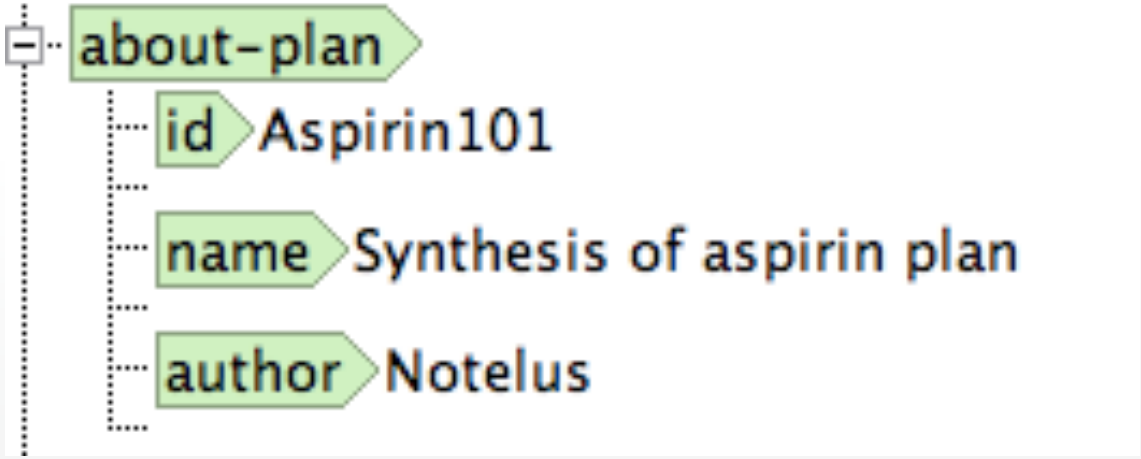
# Provenance for the plan



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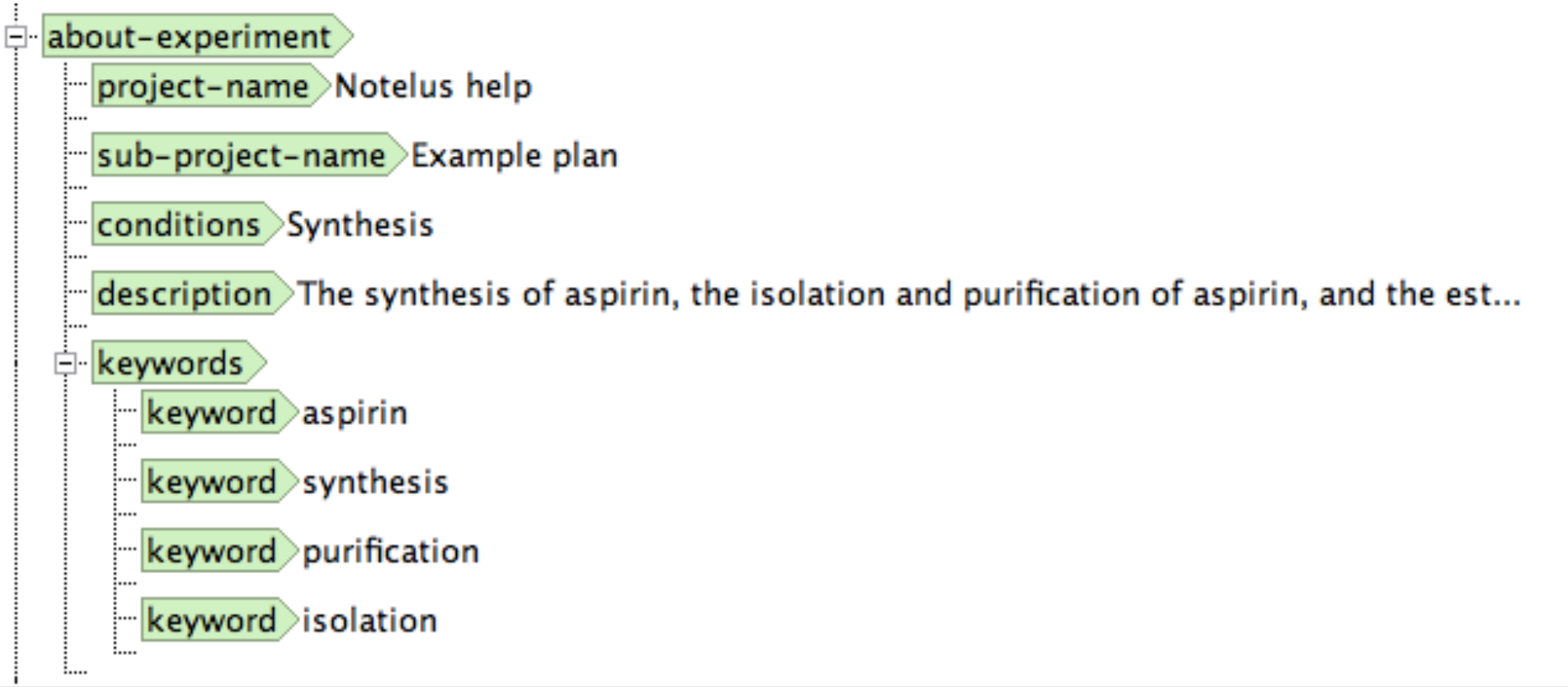
# Pre-populating information about the experiment



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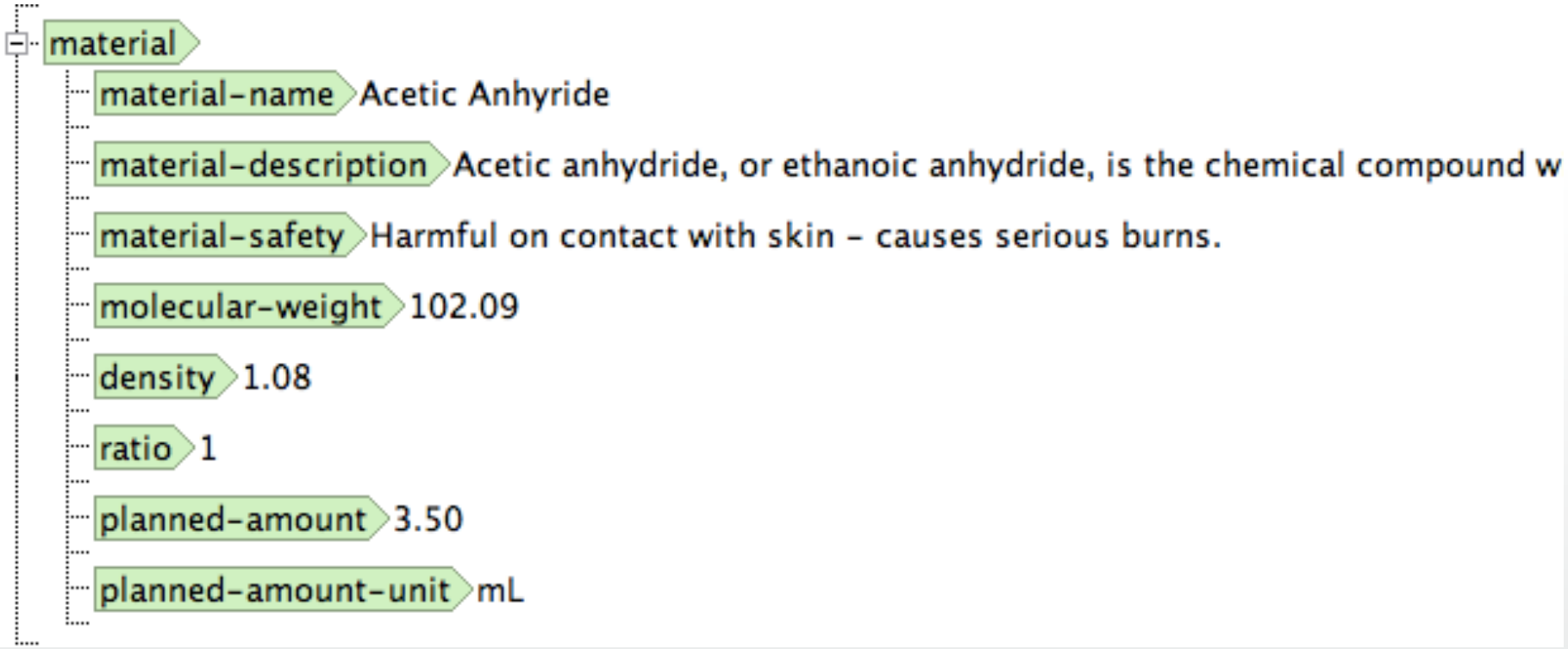
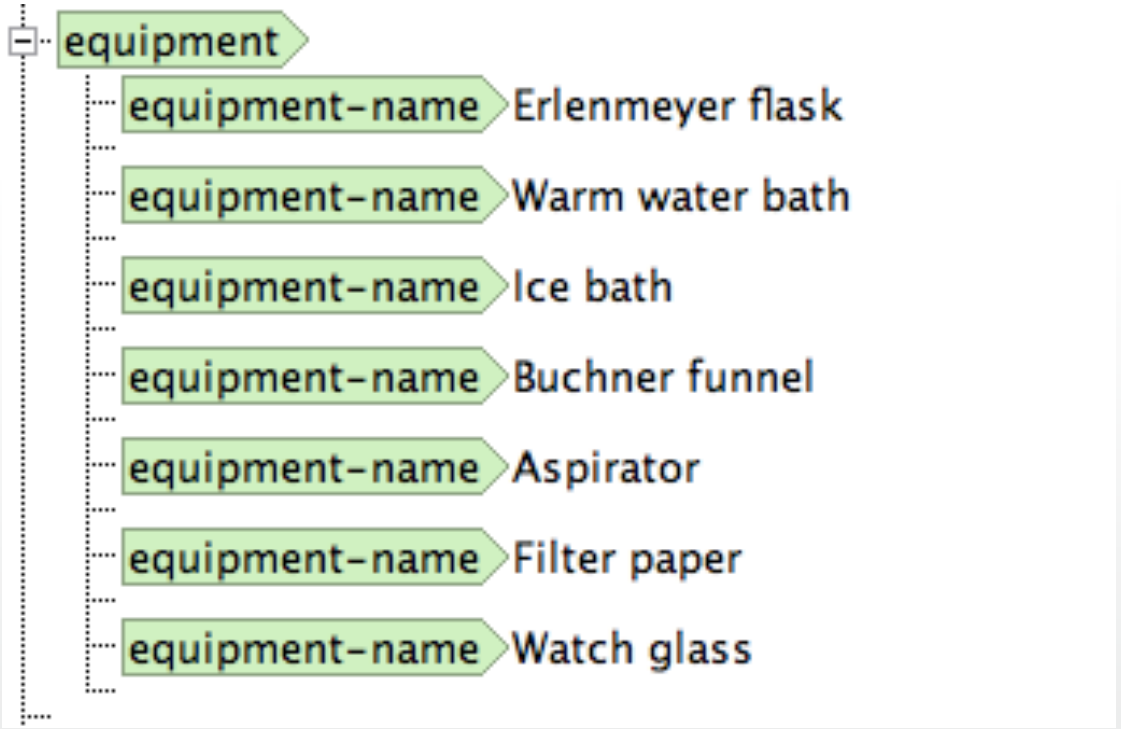
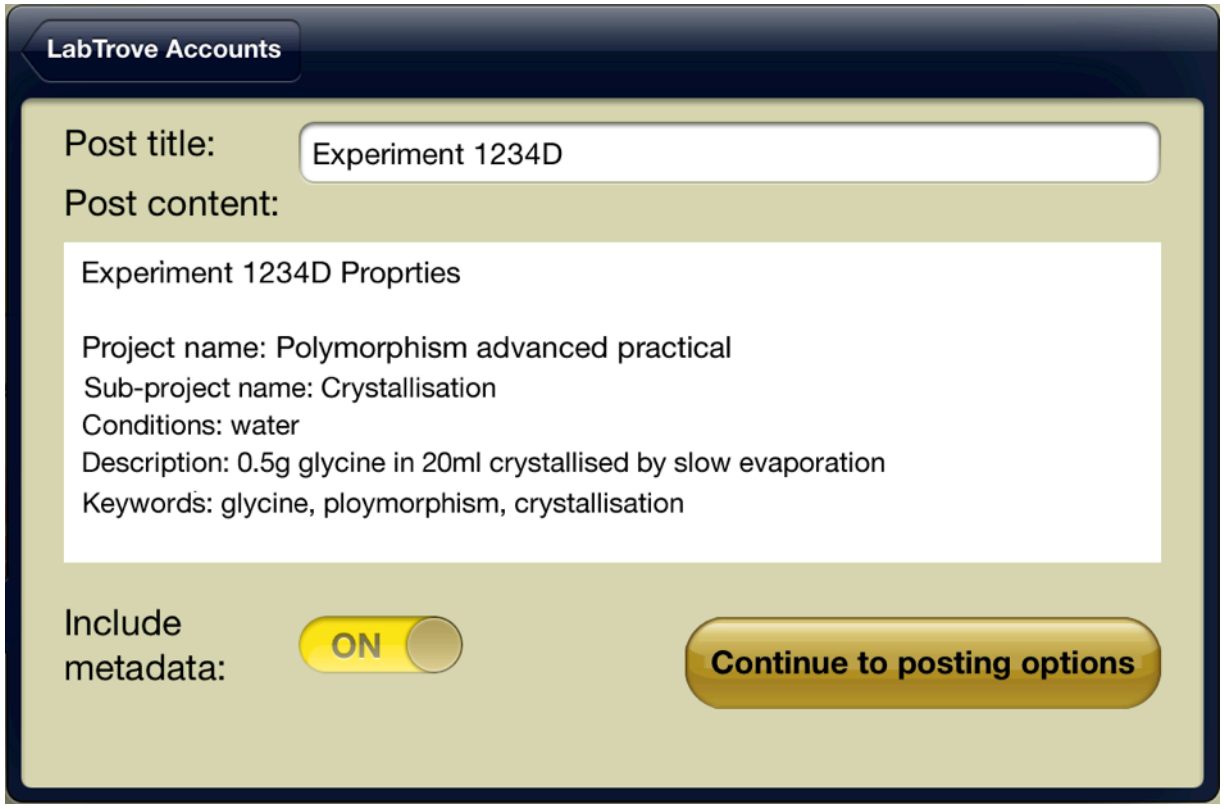
# Materials



# Equipment


equipment
equipment-name
Erlenmeyer flask
equipment-name
Warm water bath
equipment-name
Ice bath
equipment-name
Buchner funnel
equipment-name
Aspirator
equipment-name
Filter paper
equipment-name
Watch glass

# Getting the metadata into LabTrove




**Plan Id**

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

**Plan Author**

Notelus (1)
Cerys (2)

**Material**

95% Ethanol (3)
Acetic Anhyride (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


Current user: Cerys Willoughby | Log Out

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LabTrove – Aurora

# CerysTest

What would you like to post?


Project


Background


Plan


Experiment

Data


Other

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## This Notebook

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Notebook Settings
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## Authors

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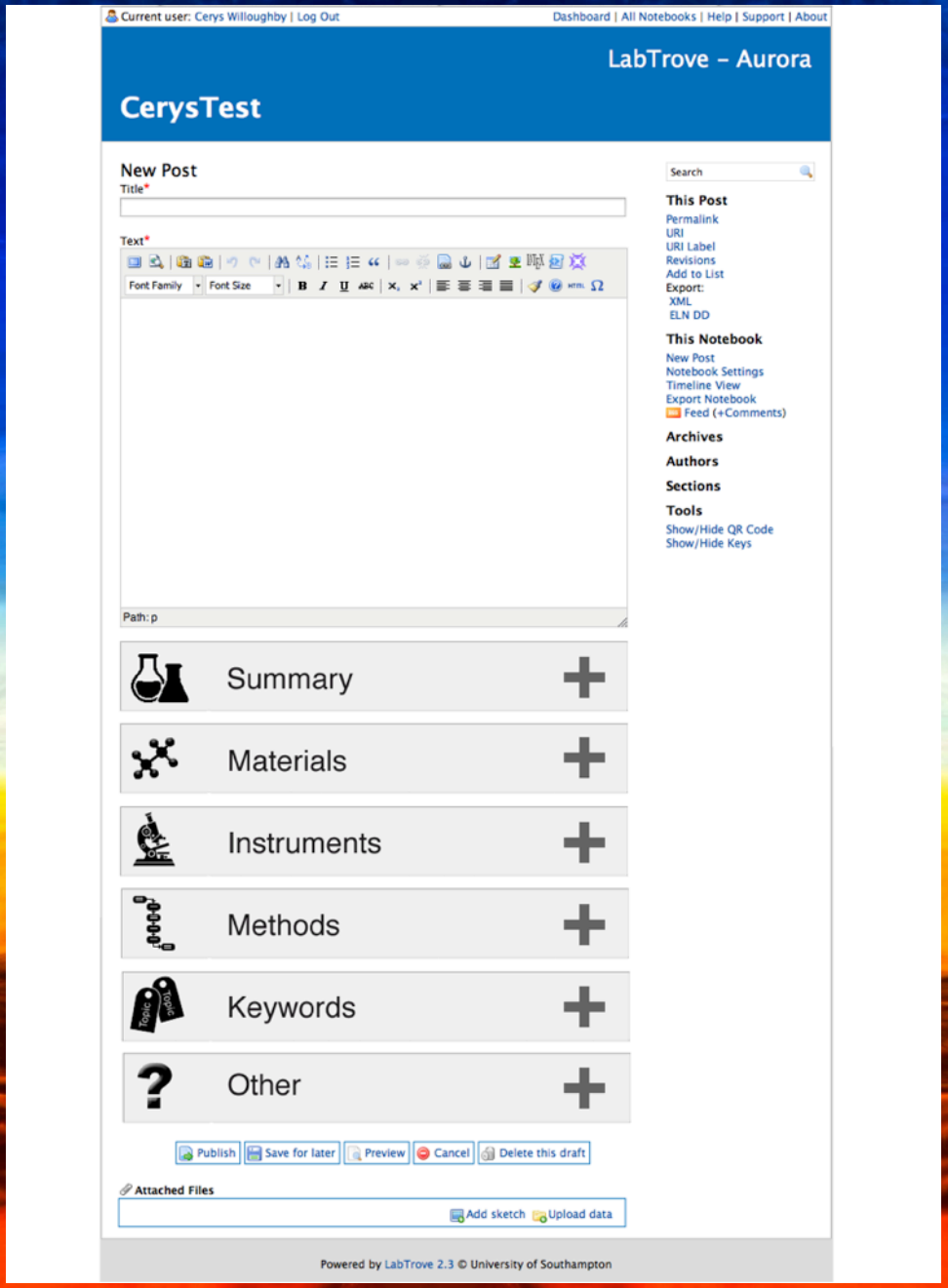
Current user: Cerys Willoughby | Log Out
Dashboard | All Notebooks | Help | Support | About
LabTrove – Aurora
CerysTest
New Post
Title*
Text*
Font Family
Font Size
Path: p
Summary
Materials
Instruments
Methods
Keywords
Other
Publish
Save for later
Preview
Cancel
Delete this draft
Attached Files
Add sketch
Upload data
Search
This Post
Permalink
URI
URI Label
Revisions
Add to List
Export:
XML
ELN DD
This Notebook
New Post
Notebook Settings
Timeline View
Export Notebook
Feed (+Comments)
Archives
Authors
Sections
Tools
Show/Hide QR Code
Show/Hide Keys
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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

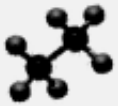
From: September — To: October

Experiment is complete

Description

Save Cancel

# Summary



# Materials

What materials are you using in your experiment?

Add

triethyl amine ✕ | 2-bromoaniline ✕ | 1-methyl-1H-pyrrole-2-carboxylic acid ✕

diethyl ether ✕ | thionyl chloride ✕

Choose from your materials

☐ Add recommended materials using ChemSpider

# Instruments

What instruments are you using in your experiment?

Add

Laser ✕ | Electrospray ✕

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/