Encouraging and Facilitating Laboratory Scientists to Curate at Source

Cerys Willoughby & Jeremy Frey
I’m recovering from a brain injury

Sometimes my words don’t work!
From paper notebooks to Digital Research Notebooks
Community Studies & Metadata Survey

104 notebooks
Effects of different interfaces for capturing information

• Standard structure
  – Get what we ask for.. (cues)

.. but some potential problems:
change of style and a loss of information (change of perspective?)
Different ways to encourage metadata generation

Free recall

Change perspective

Cues
Online Metadata Study

Photographs

Structured text

Unstructured text

Lego Rocket Cars Study

When the tablets are dissolved in water, the sodium bicarbonate reacts with citric acid (C6H8O7) to form trisodium citrate (Na3C6H5O7).

Organic Chemistry Summer School
Remote Experiments Study

117 undergraduates

Beer Law

Cued recall

Free recall

Cued recall

Free recall

Viscosity

Gas Law

Cued recall

Changing perspective
What did we learn?

Personal / Social metadata:
- Topics
- Questions
- Feelings
- Problems
- Personal
- Some consistency
- Opinions
- Statements
- Worries
- Consistent
- Limited terms
- Search strings
- Change perspective
- Topics
- Limited terms
- Search strings
- Websites
- Terms useful for search
- Tips
- Formats

Retrieval:

Free recall:
- More responses for some cues than could derived from write-up
- Some personal
- Many terms
- Get what you ask for
- No responses for certain topics when cue is missing
- Topics determined by cue
- More descriptive
- Most diverse
- Personal and guesses when question is ambiguous

Cued recall:

Chemicals, naming, and data mining:
Inviting users to add metadata

Making use of the metadata
Editing 1 photo:

On the bike
Add a description

Add tags
Separate tags with a space

Add people

Add to sets

Add to groups

Owner settings
- None (All rights reserved)
- Visible to everyone

Tags
- sunset
- landscape
- doodle
- art
- acrylics
- toto

click a tag: 2012, animals, archaeology, autumn, berlin, be, cats, cleveland, dig, dinnington, doodle, eb, eb2008, eclipse, england, expo, extremeblue, f1, florida, flower, flowers, g7, gardens, green, hampshire, hillers, history, honeymoon, hursley, hursley60, iphone, japan, july, keukenhof, kimahri, landscape, lego, legoland, macro, marwell, may, me, moscow, nature, niigata, ohio, orlando, panto, paris, phil, picnic, pink, portrait, red, roman, sc7, silverstone, spring, sunset, sydney, team, tree, ut, utpicnic, villa, water, wedding, winchester, windsor, xmas, yellow

get more of your tags | get all of your tags.
Separate each tag with a space: cameraphone, urban, moblog. Or to join 2 words together in one tag, use double quotes: "daily commute".
Curation @ source: making use of plans

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 60°C and allow to slow evaporation
Keywords: glycine, polymorphism, crystallisation

LabTrove Accounts

Post title: Experiment 1234D
Post content:

Experiment 1234D Properties
Project name: Polymorphism advanced practical
Sub-project name: Crystallisation
Conditions: water
Description: 0.5g glycine in 20ml crystallised by slow evaporation
Keywords: glycine, polymorphism, crystallisation

Include metadata: ON

Continue to posting options
Experiment Profiles

Experiment title

Summary

Experiment ID: What is your Experiment ID?

Description: Provide a short description of your experiment.

Aims: What are the aims of the experiment?

Project: Project

Start Date: 01/03/2016  End Date: 01/03/2016

Experiment is: not started

Plan

Reaction Scheme

Materials

Conditions

Instruments

Results & Analysis

Resources

What reaction scheme are you using in your experiment?

Include structure from ChemSpider

What materials are you using in your experiment?

Search Names, Registry numbers, SMILES, or InChI

Add from...

Citric acid

Molecular Formula: C6H8O7

Average mass: 192.124 Da

SMILES: O=C(=O)OCC(=O)O

Std. InChI: InChI=1/C6H8O7/c7-3(8)1-4(9,10)(11,12)13-5(15)d7-1-5/h1-7H1

Properties:

Hazard: Skin irritant, Respiratory tract irritant

Safety: Add details of safety spill, and disposal information

Planned quantity: 15.0g

Actual quantity: 167.0mg

Sodium bicarbonate

Molecular Formula: NaHCO3

Properties:
Profiles and customisation

- Reagent
- Strain
- Product
- Chemical
- Substance
- Molecule
- Batch
- Organism
- Compound
- Sample
- Input
How do we encourage researchers to curate @ source?

• Metadata has to be present to be useful!

• Using templates or profiles to avoid the ‘blank canvas’ effect and encourage metadata generation

• Ask the right questions

• Avoiding minimal metadata by banishing default values

• Use of plans to encourage early curation

• Using vocabularies if appropriate

• Data management education and support

• Functionality to make good use of metadata
Thanks for listening!
I’m recovering from a brain injury

Sometimes my words don’t work!
Smart Tea

LabTrove

Enantioselective Hydrogenation of dehydro-PZQ and derivatives

Preparation of MNR40-2

Materials

Procedures

Samples
Remote Experiments Study - Viscosity

117 undergraduates

Free recall

Changing perspective

Cued recall
Remote Experiments Study – Gas Law

Free recall

Changing perspective

Cued recall
Remote Experiments Study – Beer Law

Free recall

Changing perspective

Cued recall