



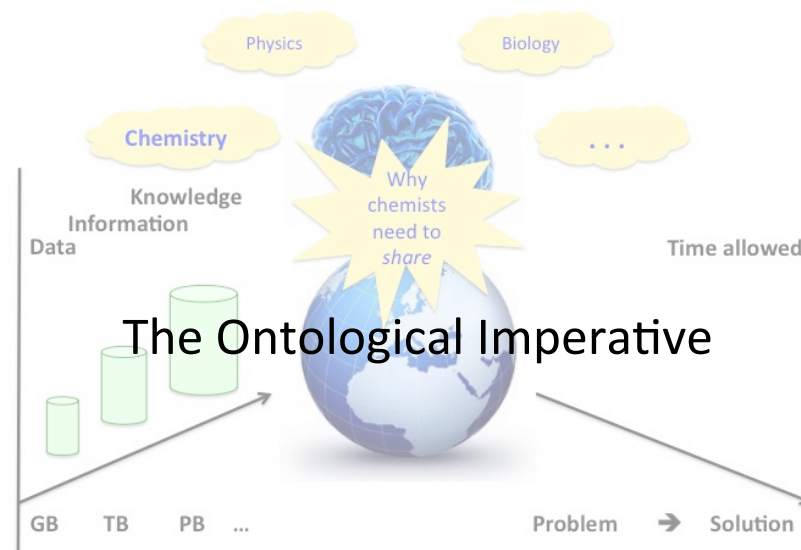
## Sample management with the LabTrove ELN

Jeremy Frey, Simon Coles, Colin Bird,  
Andrew Milsted, John Robinson, David  
Newman, Tim Parkinson, Cameron Neylon,  
Jenny Hale, Graham Tizzard, Jon Blower

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## Kant's Categorical Imperative

- Kant's version of duty-based ethics
- A 'categorical imperative' is a rule that is true in all circumstances.
  - BBC Ethics Web Pages
- *Self evidently true and a good thing*



Immanuel Kant © wikipedia

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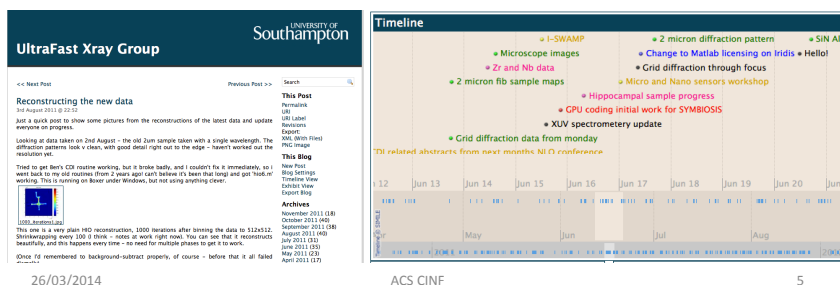
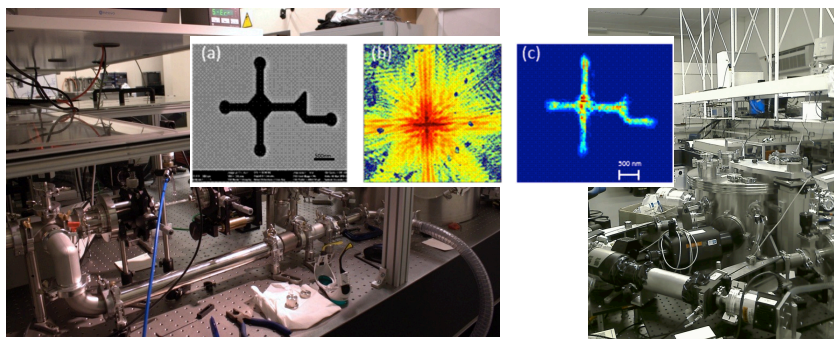
3

**I STILL DO SOME CHEMISTRY!**

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## Sample Tracking Scenarios

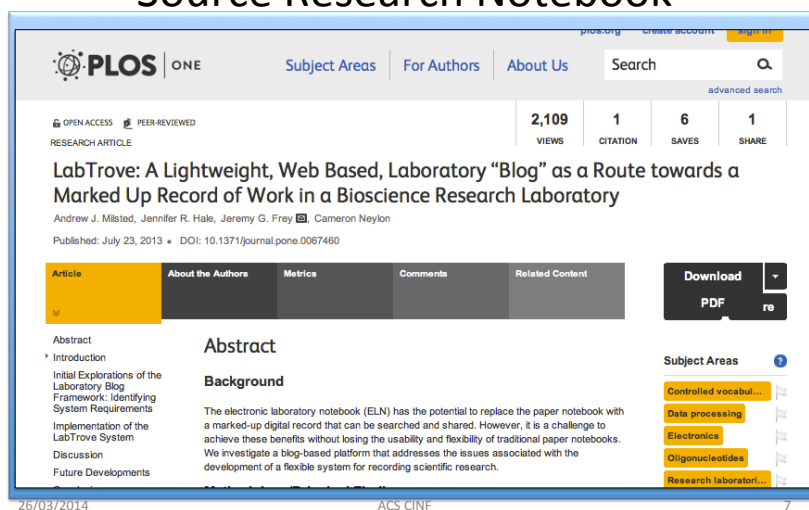
- Keeping track of separate samples and demonstrating reproducibility between batches of sample;
- Maintaining links between samples, experiment data, derived data, and subsequent publications;
- Using a combination of URI and barcodes to provide both ready identification of specific items and a simple sample management system, with no additional effort.

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## LabTrove Researcher Centric Open Source Research Notebook



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## Linking

- retain the journal characteristics of traditional notebooks
- exploiting the potential for linking together
  - procedures,
  - materials,
  - samples,
  - observations,
  - data, and analysis reports.

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# Links and URI

- Each data file added to the Trove has its own URI
- LabTrove preserves the provenance by maintaining links between the objects in notebooks
- Enabling users to capture the appropriate metadata.
- Links and metadata can be used individually or in combination to enable selective retrieval.

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LabTrove – Aurora

IDCC Test

IDCC Conference Test Demo

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Search

Plan for the experiment

17th March 2014 @ 02:05

Following ideas from [First Thoughts about a new experiment](#)

Plans

1. design flow cell

2. order graphene

3. Assemble and test flow cell

4. Attempt x-ray microscopy with graphene cell

This post is linked by:

Graphene windows

Linked Posts

This post is linked by:

Graphene windows

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March 2014 (3)

February 2014 (4)

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IFTTT

Andy Stanford-Clark @andysc · 11h

Ferry journeys SO much more productive when you have internets :) bug raised, pothole reported, red nodes updated :) [Expand](#)

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Andy Stanford-Clark @andysc · 12h

received backlog of 24 daily balance txts from @CitibankUK . Hint - clear the transmission queue before restarting! [#schoolboyerror](#) [Expand](#)

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Jeremy Frey @profechem · 16h

Graphene windows [ift.tt/1ITgrue](#) [Expand](#)

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Jeremy Frey @profechem · 16h

Plan for the experiment [ift.tt/1ITgru4](#) [Expand](#)

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First Thoughts about a new experiment [ift.tt/1oeWCMN](#) [Expand](#)

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Retweeted by CameronNeylon

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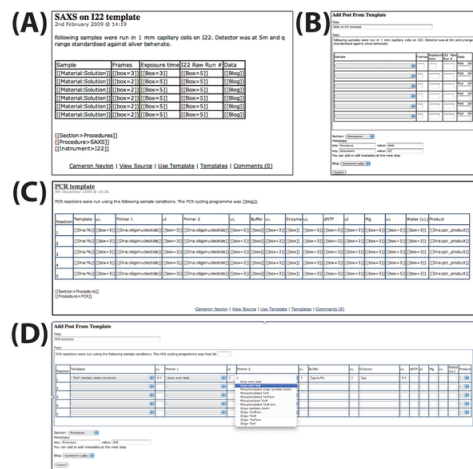
11

Figure 4. Diagram illustrating the alternative schemes for determining which research objects merit their own posts.

Milsted AJ, Hale JR, Frey JG, Neylon C (2013) LabTrove: A Lightweight, Web Based, Laboratory "Blog" as a Route towards a Marked Up Record of Work in a Bioscience Research Laboratory. PLoS ONE 8(7): e67460. doi:10.1371/journal.pone.0067460 <http://www.plosone.org/article/info:doi/10.1371/journal.pone.0067460>

PLOS ONE

Figure 6. Extracts illustrating the design and use of templates.



Milsted AJ, Hale JR, Frey JG, Neylon C (2013) LabTrove: A Lightweight, Web Based, Laboratory "Blog" as a Route towards a Marked Up Record of Work in a Bioscience Research Laboratory. PLoS ONE 8(7): e67460. doi:10.1371/journal.pone.0067460  
<http://www.plosone.org/article/info:doi/10.1371/journal.pone.0067460>

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## TEMPLATES

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## Sequence of process

### T4 DNA ligase 29.09.08

29th September 2008 @ 11:08

Post Type: Enzyme

Property	Data
Name	T4 DNA Ligase
Supplier	Promega
Batch Number	19827739
Expiry	03.09.2010
Cutting Sequence	N/A
Storage Buffer	10 mM Tris-HCl (pH 7.4 @ 25°C)
2	50 mM KCl
3	1 mM DTT
4	0.1 mM EDTA
5	50% Glycerol
6	

This Post is Linked By: Ligation 5025/99 (Experiment 3 (large), r 5025/111 (experiment 3 round 1); Test ligations 5025/113 (experim 1); Ligation 5025/116 (experiment 3)

Jennifer Hale | View Source | Ms

### T4 DNA ligase buffer 29.09.08

29th September 2008 @ 11:09

Post Type: Buffer

Property	Data
Name	T4 DNA Ligase
Supplier	Promega
Batch Number	550815
Expiry	03.09.2010
pH	None given
Ingredients	100 mM Tris-HCl (pH 7.8 @ 25°C)
2	100 mM MgCl <sub>2</sub>
3	100 mM DTT
4	10 mM ATP
5	
6	

this buffer has been separated into 10 µL aliquots  
This Post is Linked By: Ligation 5025/99 (Experiment 3 (large), r 5025/111 (experiment 3 round 1); Test ligations 5025/113 (experim 1); Ligation 5025/116 (experiment 3)

Jennifer Hale | View Source

### Ligation 5025/99 (Experiment 3 (large), round 1)

29th September 2008 @ 11:17

Post Type: Ligation

Post assessment: Ligation (DNA assessment)

Reaction	Insert	µl Backbone	µl Buffer	µl Water	µl Enzyme	µl Product
1	Purified 5025/95 (L1, B1)	Purified 5025/95 (L1, B1)	10 mM Tris-HCl (pH 7.4 @ 25°C)	None	10 mM Tris-HCl (pH 7.4 @ 25°C)	Ligation 5025/99 (Experiment 3 (large), round 1)
2	Purified 5025/95 (L1, B1)	Purified 5025/95 (L1, B1)	10 mM Tris-HCl (pH 7.4 @ 25°C)	10 mM Tris-HCl (pH 7.4 @ 25°C)	10 mM Tris-HCl (pH 7.4 @ 25°C)	Ligation 5025/99 (Experiment 3 (large), round 1)
3	Purified 5025/95 (L1, B1)	Purified 5025/95 (L1, B1)	10 mM Tris-HCl (pH 7.4 @ 25°C)	10 mM Tris-HCl (pH 7.4 @ 25°C)	10 mM Tris-HCl (pH 7.4 @ 25°C)	Ligation 5025/99 (Experiment 3 (large), round 1)

Ligations were set up as listed in 200 µL tubes and incubated at room temperature for 2 hours to give the products listed.

Jennifer Hale | View Source | Procedure | Comments (0)

## Links!

### Purified 5025/95 digestion product (E3 (L1), R1)

25th September 2008 @ 14:05

Post Type: DNA gel product

50 µL of purified digestion products from Digestion 5025/95 (Experiment 3 (large), round 1); Ligation 5025/99 (Experiment 3 (large), round 1); DNA gel to check at

Jennifer Hale | View Source | Product | C

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## Links & Index

Round 2 mutagenesis on plasmid 4880/35 (4880/36)  
Digestion of 4880/36 using EcoRI and NcoI (4880/37)  
Ligation of 4880/37 into pBAD/His method 2 (Lyo-Ligase™) (4880/39.2) and Ligation of 4880/37 into pBAD/His method 1 (4880/39.1)  
Transformation of plasmids 4880/39.1 and 4880/39.2 into XL1 blue (4880/40)  
Electroporation of 4880/40 into BW25141 (4880/41)  
X-glu assay of electroporation 4880/41  
Plasmid preparation from electroporations 4880/41.1-4

### Round 3

Digestion of 4880/42 (4880/43)  
Ligation of 4880/43 into pBAD/His (4880/44), Ligation of 4880/43 into pBAD/His (4880/49) and Test ligation conditions (4880/46)  
Transformation of 4880/44 into XL1 Blue (4880/45), Transformation of 4880/46 into XL1 Blue (4880/47) and Transformation of 4880/49 into XL1 Blue (4880/50)  
Electroporation: repeat of 4880/51 and 4880/52 (4880/53)  
X-glu and X-gal assays for electroporation 4880/53

### Round 4

R4 Mutagenesis 5025/11  
Digestion 5025/14 - round 4  
Ligation 5025/15 - round 4  
Transformation 5025/16 (round 4) and Transformation 5025/17 - round 4  
Electroporation 5025/18 (round 4)

### Library 4

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Investigations into neutral drift

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Search

Template: Analysis of solubilities for usefulchem

15th September 2008 @ 12:58

Post Type: Usefulchem

Tube Number	Residue Name	Residue Mass	Solid RMM	mmol Solid in Solution	Molarity
81	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
82	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
83	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
84	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
85	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
86	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
87	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
88	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
89	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
810	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
811	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
812	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
813	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
814	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
815	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
816	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
817	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
818	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
819	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]
820	[[Post_Type:Residue]]	[[box]]	[[box]]	[[box]]	[[box]]

This Blog

New Post

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January 2013 (1)

July 2012 (3)

June 2012 (1)

May 2012 (3)

May 2010 (1)

November 2009 (1)

September 2009 (1)

August 2009 (1)

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Authors

Error (3)

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Summary (1)

Templates (32)

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DNA Gel Product (130)

Investigations into neutral drift

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Search

Transformation 5025/117

11th November 2008 @ 13:26

Post Type: Transformation

Risk assessment: Transformation risk assessment

Reaction	Cells	μL	Plasmid	μL	Product
1	New Supercompetent XL1 BLue	40	Ligation product 1	5025/116 2	Transformation 5025/117 plate 1
2	New Supercompetent XL1 BLue	40	Ligation product 1	5025/116 2	Transformation 5025/117 plate 2
3	New Supercompetent XL1 BLue	40	Ligation product 1	5025/116 2	Transformation 5025/117 plate 3
4	New Supercompetent XL1 BLue	40	Ligation product 1	5025/116 2	Transformation 5025/117 plate 4
5	New Supercompetent XL1 BLue	40	Ligation product 1	5025/116 2	Transformation 5025/117 plate 5
6	New Supercompetent XL1 BLue	15	p042 (27/9/07)	1	Transformation 5025/117 plate 6 (+ve ctrl)
7	New Supercompetent XL1 BLue	15	None	0	Transformation 5025/117 plate 7 (-ve ctrl)

Cells, 15 mL Falcon tubes, p042 and ligations were cooled on ice whilst LB amp plates and SOC medium\* were warmed to 37°C.  
Transformations were set up as listed and cooled over ice for a further 30 minutes.  
The transformants were heat shocked in a waterbath at 42°C for 45 seconds then immediately transferred to ice for 2 minutes. SOC medium (250 μL) was added to each transformant then the transformants incubated at 37°C for 1 hour.  
750 μL was added to LB amp plates and incubated at 37°C overnight

This Blog

New Post

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Archives

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Error (237)

Sections

Materials (90)

Notes (48)

Procedure (405)

Product (1578)

Safety (11)

Summary (1)

Templates (32)

Post Type

DNA Gel Product (130)

11:31

blogs.chem.soton.ac.uk

Mathematical P... A New Thermod... The Journal of... Open-System N... Microsoft Word... Knowledge Eng... Scientists Disco... Investigation...

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UNIVERSITY OF Southampton

## Investigations into neutral drift

### Add Post From Template

Title\*  
Template: Analysis of solubilities for usefulchem

Text\*

Tube Number	Residue Name	Residue Mass	Solid RMM
B1			
B2			
B3			
B4			
B5			
B6			

11:31

blogs.chem.soton.ac.uk

Mathematical Open-System N... Microsoft Word... Knowledge Eng... Scientists Disco... Investigation...

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UNIVERSITY OF Southampton

Investigations into neutral drift

Add Post From Template

Title\*

Template: Analysis of solubilities for usefulchem

Text\*

NaCl residue from THF

Residue Mass

Solid RMM

5025/96 NaCl residue from THF

5025/96 NaCl residue from ethanol

5025/96 NaCl residue from methanol

5025/96 Mannitol residue from THF

5025/96 Mannitol residue from ethanol

5025/96 Mannitol residue from methanol

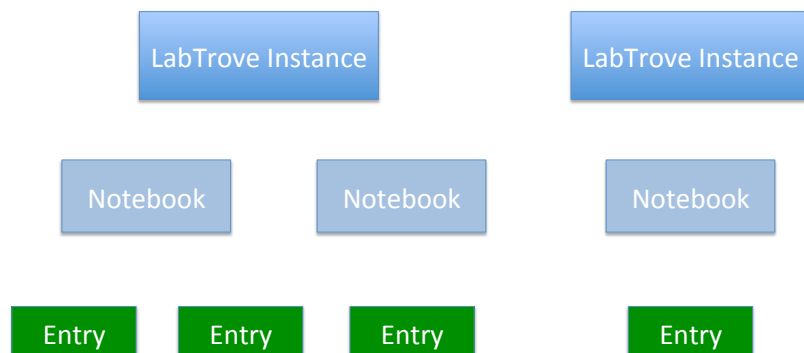
5025/96 Glucose residue from THF

5025/96 Glucose residue from ethanol

5025/96 Glucose residue from methanol

Tube Number	Residue Name	Residue Mass	Solid RMM
B1			
B2			
B3			
B4			
B5			
B6			

## Linking and Linking Back



Linking and re-verse link/cite/track back between all of these is possible

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### Graphene windows

17th March 2014 @ 02:08

Sample: graphene  
Sample No: 1

The details of the graphene windows arrived 16 March 2014

10 slides of graphene on SiN, single layer graphene, 0.3 nm thick, 2 x 2 micron squares for experiments Plan for the experiment

Jeremy Frey | View Source | samples | Comments (0)

Uri: <http://aurora.labtrove.org/uri/434>

Key: e246585952eb5159b2803299fa1edc55

Last Updated: 17th March 2014 @ 02:11

### Chemspider Info

graphene | SiN

graphene (Confidence: 0.65708, Timestamp: 2014-03-17 02:11:24)

### QR Code



Search URI

### This Post

Permalink

URI

URI Label

Revisions

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Item Manifest

### Archives

March 2014 (3)

February 2014 (4)

### Authors

Jeremy Frey (7)

### Sections

Conference (3)

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Test (1)

### Nmr

H (1)

### Materials

Graphene (1)

### Sample

Graphene (1)

### Sample No

1 (1)

### Tools

Show/Hide QR Code

Show/Hide Keys

### QR Code

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Linking the Physical and Digital worlds

## SAMPLE TRACKING

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## Demonstrating reproducibility

- Demonstrating reproducibility between batches of sample was an important aspect of this collaboration
- relied on the linking and classification features of LabTrove.
- Analyses of coated surfaces could be linked to the separate batches and also to the master entry for all the batches,
- enabling the project to keep track of separate samples
- to see the overall picture in terms of surface comparison and reproducibility.

26/03/2014

26/03/2014

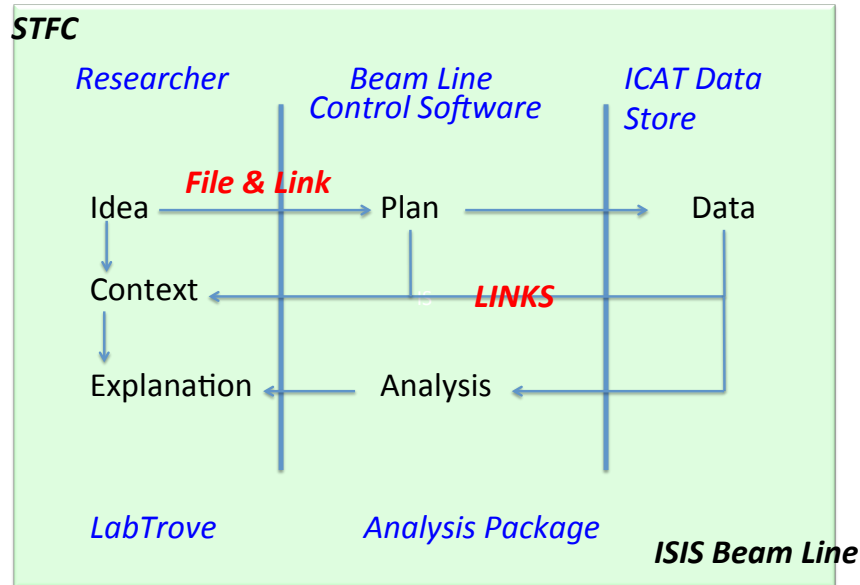
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## ISIS – NEUTRON FACILITY

## Large Facility Users (ISIS)

- ISIS Facility Provides
  - Experiment control file
  - Automated equipment
  - Data storage infrastructure
  - Analysis packages provided
- LabTrove Provides
  - The data provenance i.e links between
  - Samples, sample information
  - experiment data,
  - derived data, and subsequent publications.



## AutoTrove from Matlab

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

blogs@xray

Older Posts >> Search

**This Blog**  
New Post

**ion\_vs\_spot.m**  
14th May 2012 @ 11:59

```

matlab coder
%ion_vs_spot
% 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 = 30.5; % 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)] = adx8
end
cutoff_lambda = lambda ./cutoff_h
  
```

Figure 1  
Published with MATLAB® 7.11.1

Computational processes also blog

William Brocklesby | View Source



# Data Citation

Supplementary data linked to laboratory notebooks

## DATA CITATION

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# Data Citation

## Metadata Search beta

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36 documents found in 132ms  
Page 1 of 4

**Type**

**Year**

**Year**

(3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one  
doi:10.5258/POC/LT/R/1  
Graham Tizzard • Nicola Knight  
creator: [Graham Tizzard](#)

(3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one  
doi:10.5258/POC/LT/R/2  
Graham Tizzard • Nicola Knight  
creator: [Graham Tizzard](#)

(3E)-3-(4-Methoxybenzylidene)-1,3-dihydro-2H-indol-2-one  
doi:10.5258/POC/LT/R/3  
Graham Tizzard • Nicola Knight  
creator: [Graham Tizzard](#)

(3E)-3-(4-Methylbenzylidene)-1,3-dihydro-2H-indol-2-one  
doi:10.5258/POC/LT/R/4  
Graham Tizzard • Nicola Knight  
creator: [Graham Tizzard](#)

(3E)-3-(4-Nitrobenzylidene)-1,3-dihydro-2H-indol-2-one  
doi:10.5258/POC/LT/R/5  
Graham Tizzard • Nicola Knight  
creator: [Graham Tizzard](#)

[doi.org/10.5258/POC/LT/R/1](#)

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Helping you to find,  
access, and reuse data

**DataCite**

### Invitation to tender for the new DataCite website

Published by Sergio Ruiz on 10 March 2014 - 8:56am

Following our [Strategy for 2013-2016](#) DataCite is working on the creation of a new website. Firms and professionals are invited to submit a proposal. You will find all the details [in this document](#).

Tags:  
[datacite](#), [tender](#), [website](#)  
[Read more](#)

### DataCite Strategy 2013-2016

Published by Sergio Ruiz on 3 March 2014 - 11:00am

[Why cite data?](#)  
[What is DataCite?](#)  
[What do we do?](#)

**members**

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# Data Citation

## DataCite Content Service Beta

### 10.5258/POC/LT/R/1

presents DataCite's metadata for [doi:10.5258/POC/LT/R/1](#).

g page of this dataset please follow <http://dx.doi.org/10.5258/POC/LT/R/1>

Graham Tizzard; Nicola Knight; (2013): (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one; LabTrove - Univ  
Southampton. <http://dx.doi.org/10.5258/POC/LT/R/1> [RIS](#) [BibTeX](#)

### Identifiers

<http://poc.labtrove.soton.ac.uk/report/1>

### Formats

[text/html](#)  
[application/x-datacite+xml](#)  
[application/vnd.datacite.datacite+xml](#)

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## Data Citation

### Reports

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

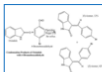
Graham Tizzard, Nicola Knight  
13th June 2013 | doi:10.5258/poc/lt/r/1

**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



Condensation Product of Oxindole with 4-Bromobenzaldehyde

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

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## Data Citation

### Synthesis of 4-substituted methyldene oxindoles

Project E-Lab Notebook for the synthesis of five 4-substituted methyldene oxindole from oxindole and their corresponding aromatic aldehydes.

<< Next Post

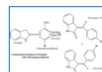
Previous Post >>

Search

Condensation Product of Oxindole with 4-Bromobenzaldehyde

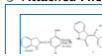
11th March 2012 @ 14:47

Substituent: Bromo



Condensation Product of Oxindole with 4-Bromobenzaldehyde

Attached Files



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**Archives**  
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April 2012 (15)  
March 2012 (29)

**Authors**  
Nicola Knight (44)  
Graham Tizzard (1)

26/03/2014

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## Thanks & Acknowledgements

- UK e-Science & Digital Economy Programmes
- RCUK: EPSRC, BBSRC & TSB, JISC/HEFCE, Microsoft & IBM, for funding and support
- Southampton Colleagues and Students from Chemistry, Electronics & Computer Science, Engineering, Mathematics/Statistics, iSolutions and the Library
- Colleagues at Bath/UKOLN, Oxford/OERC, STFC, Reading, Penn State, Cornell, PNNL, UNSW, USyd



## "T'ain't what you do (it's the way that you do it)"

James Young and Sy Oliver (1939)



Trust me Mort - no electronic communications superhighway, no matter how vast and sophisticated, will ever replace the art of the schmooze