

Towards a global open scientific notebook infrastructure

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Cerys Willoughby, Cameron Neylon &
Matthew Todd



Science as an open enterprise

June 2012

THE
ROYAL
SOCIETY

EC042_pA4158
pic-EC042_pA4035
EC042_pA4032
SIGA-EC042_pA4035



Digital Research Data Sharing and Management

December 2011

Science is increasingly interdisciplinary



because good research needs good data

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In this section

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The coverage of funders' publication and data policies



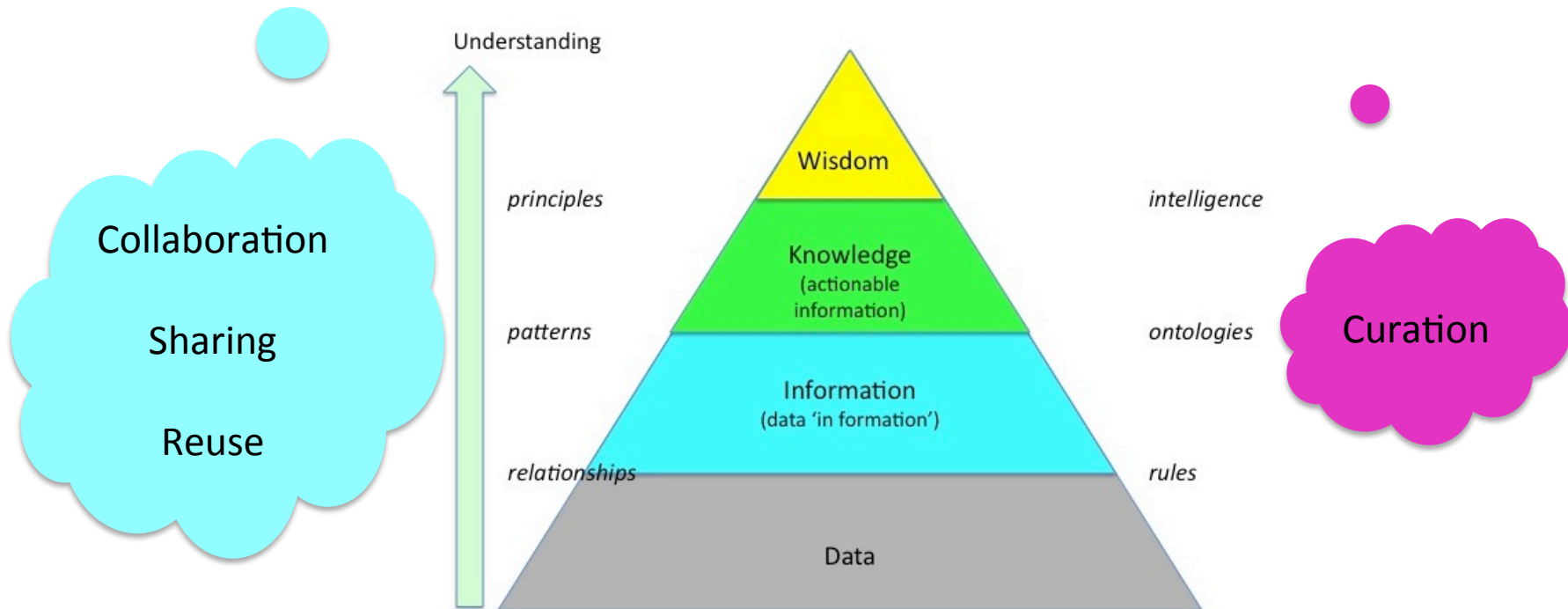
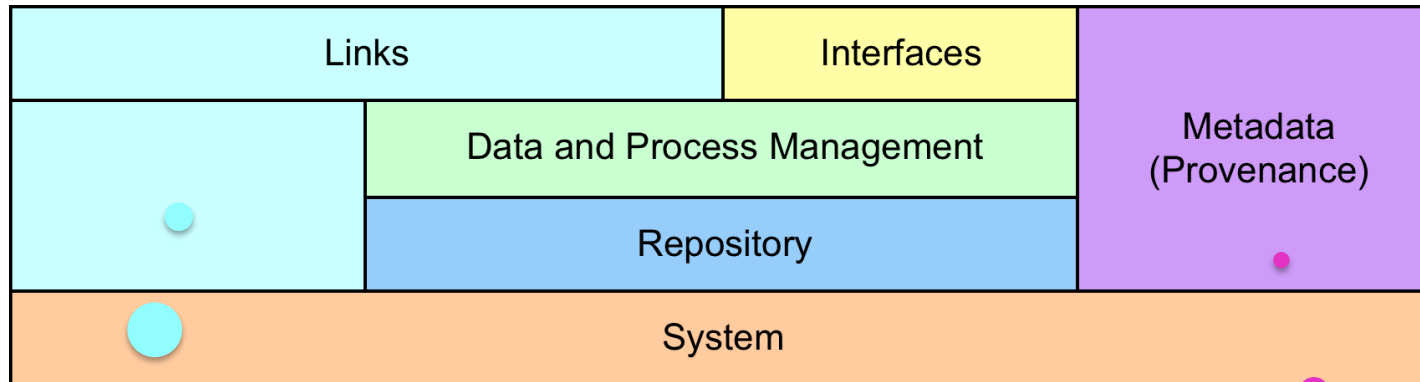
EUROPEAN COMMISSION

PRESS RELEASE

Brussels, 17 July 2012

Scientific data: open access to research results will boost Europe's innovation capacity

Infrastructures - Architecture



Comparison with
traditional paper
notebooks

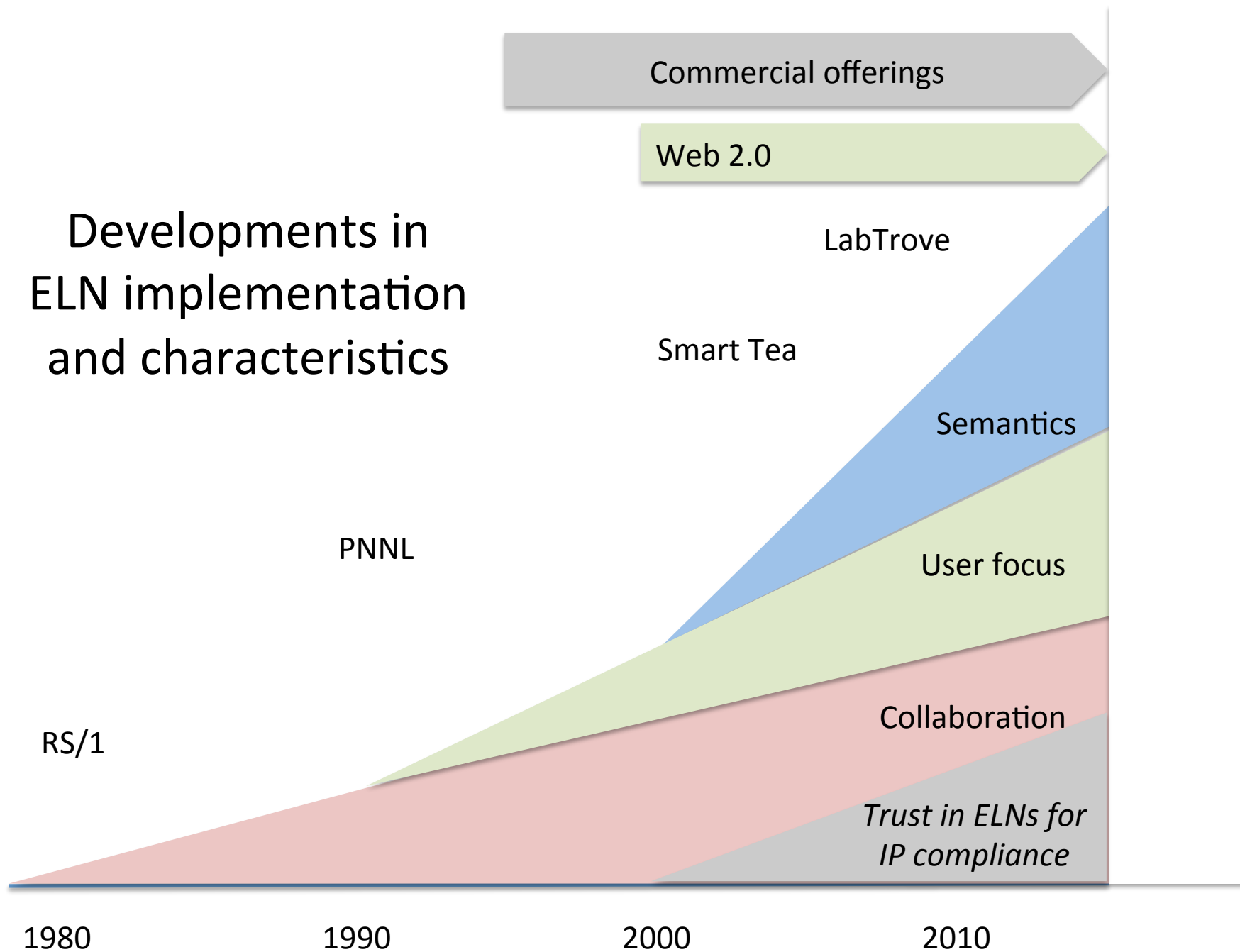
Electronic Laboratory Notebooks

ELNs

Communication
Collaboration
Sharing
Linking
Curating

- Higher Quality Record
- Natural linking to data and external resources
- Easier Collaboration
- Improved planning
- Improved discussions
- Efficiency gain in production of presentations/reports
- Change the nature of Professor/Student interactions

Developments in ELN implementation and characteristics



The LabTrove story



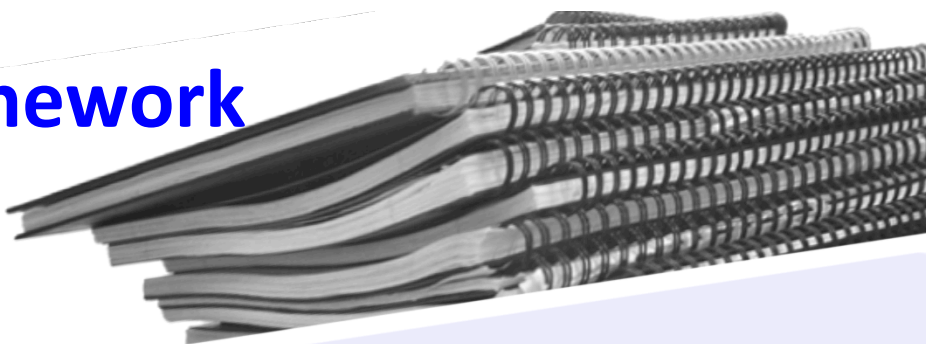
The screenshot displays the LabTrove website interface. At the top, a blue banner features the "LabTrove" logo in white. Below this, a large image shows a close-up of a laboratory notebook with the text "preserving the record" overlaid in blue. The left sidebar contains a list of navigation links: About Us, Get LabTrove, Documentation, Support, Publications, Users, and Contact Us. The main content area is titled "our experiment" and features a post about the "Pictet-Spengler route to Praziquantel". This post includes a chemical reaction scheme showing the conversion of a starting material to Praziquantel using MeSO₂H under various conditions. To the right of the main content, there is a "LabTrove labtrove" sidebar with three public blog posts, each providing a title, a URL, and social media interaction options like "reply", "retweet", and "favorite".

LabTrove enables the formation of a Smart Research

<http://www.labtrove.org>

Smart Research Framework

My Lab Notebook



Introduction

Introduction

Software Overview

Partners

Vision

SRF Software

LabTrove

Plan3

The SRF project is a shared virtual management.

Providing tools to meet the need for responsibility, collaboration, and use of projects and mental assets.



LabTrove

"preserving the record"

© flickr.com/julia_manzerova

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our experiment

Pictet-Spengler route to Praziquantel

Continuation: Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MWS6-9 to MWS6-12)

17th March 2011 @ 07:27

Acid-catalyzed Pictet-Spengler reaction using methanesulfonic acid (MWS6-5 to MWS6-8)

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

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LabTrove

labtrove

labtrove Public Blog Post: Synthesis of amine-linked analogue of TCMDC-123812 via reductive amination... <http://t.co/Bla5hWbb> #malaria #drugdesign

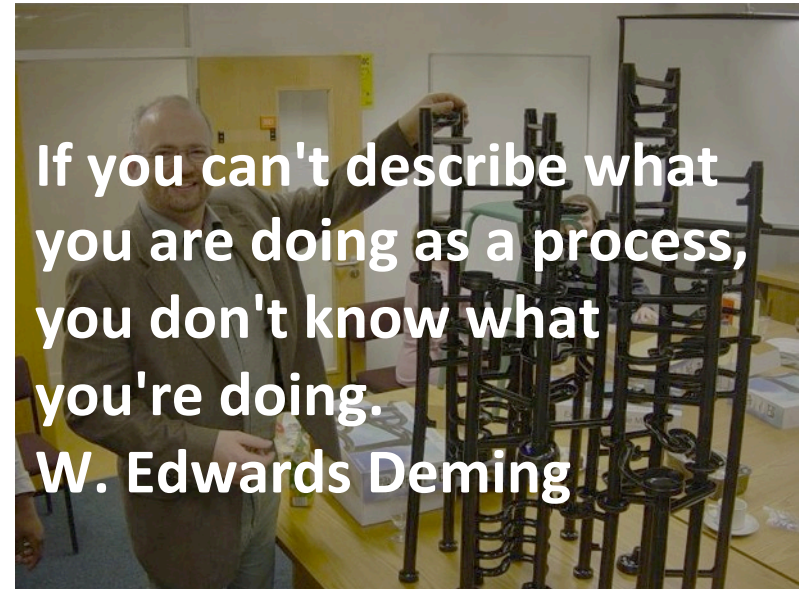
yesterday · reply · retweet · favorite

labtrove Public Blog Post: Synthesis of ether-linked analogue of TCMDC-123812 (PMY 37-1) <http://t.co/XhQyRb8i> #malaria #drugdesign

unstartrou · rmlb · entwert · favorite

How do we communicate?

- Surprisingly difficult to explain what a process involves
- Much of the detail is assumed to be understood and not explicitly discussed
- This is where the misunderstandings usually arise.



LabTrove

"preserving the record"

Transformation of plasmid JRH4712/66 into BW25141 by electroporation

11th December 2006 @ 14:31

Transformations were set up according to the following protocol: LB Ampicillin arabinose plates and SOC medium were warmed to 37 °C briefly before the arabinose plates were spread with X-glu (80 µL, 1:1 X-glu and LB) and allowed to continue warming.

BW25141 cells, plasmid JRH4712/66, p042, and electroporator cuvettes were cooled on ice. Items were added to the cuvettes as follows

| | 1 | +ve ctrl | -ve ctrl |
|-----------------|-------|----------|----------|
| BW25141 | 40 µL | 40 µL | 40 µL |
| plasmid 4712/66 | 4 µL | 0 µL | 0 µL |
| p042 | 0 µL | 4 µL | 0 µL |

Cuvettes were electroporated at 1.75 kV, immediately had SOC medium (950 µL) added and the transformant transferred to eppendorf. The transformants were diluted 1 in 20 with LB and 100 µL added to LB amp arabinose plates and incubated at 37 °C overnight.

[Pictet-Spengler route to Praziquantel](#)

Conversion: Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MSA)-9 to M956-121

Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MSA)-9

Conversion of Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MSA)-9

Lab Book Ref: jrh4712-63 (1), jrh4712-64 (2), jrh4712-66 (1), jrh4712-76 (1), jrh4712-77 (1), jrh4712-78 (1), jrh4712-80 (1), jrh4712-81 (1), jrh4712-83 (1), jrh4712-84 (1), jrh4712-85 (1), jrh4712-86 (1), jrh4712-87 (1), jrh4712-88 (1), jrh4712-89 (1), jrh4712-90 (1)

Product: jrh4712-74 (1), jrh4712-76 (1), jrh4712-76a (1)

Sample Parent: jrh4712-74 (1), jrh4712-76 (1), jrh4712-76a (1), jrh4712-77 (1), jrh4712-78 (1), jrh4712-79 (1)

[Beta-glucuronidase](#) | Comments (3)

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Lab Book Ref

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JR4712-64 (2)
JR4712-66 (1)
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jrh4712-83 (1)
jrh4712-84 (1)
jrh4712-85 (1)
jrh4712-86 (1)
jrh4712-87 (1)
jrh4712-88 (1)
jrh4712-89 (1)
jrh4712-90 (1)

Product
jrh4712-74 (1)
jrh4712-76 (1)
jrh4712-76a (1)

Sample Parent
jrh4712-74 (1)
jrh4712-76 (1)
jrh4712-76a (1)
jrh4712-77 (1)
jrh4712-78 (1)
jrh4712-79 (1)

29/01/2013

Test digestions to check the activity of two batches of EcoRI and NcoI

22nd January 2007 @ 11:57

Lab Book Ref: jrh4712-89
Sample Parent: jrh4712-80, blue
Sample Parent: jrh4712-80, white
Digestions were set up as follows:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---------------|--------|--------|---------|--------|---------|--------|--------|--------|---------|--------|----|
| - | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| 4712/80 blue | 8 µL | - | - | 8 µL | - | - | 8 µL | - | - | - | - |
| 4712/80 white | - | 8 µL | - | - | 8 µL | - | - | 8 µL | - | - | - |
| p042 | 7.5 µL | 7.5 µL | 10.5 µL | 7.5 µL | 10.5 µL | 10 µL | 7.5 µL | 7.5 µL | 10.5 µL | 10 µL | - |
| water | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | - |
| EcoRI buffer | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | - |
| NEB buffer | - | - | - | - | - | - | - | - | - | - | - |
| BSA | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | 2 µL | - |
| EcoRI (a) | 0.5 µL | 0.5 µL | 0.5 µL | 0.5 µL | 0.5 µL | 0.5 µL | 0.5 µL | 0.5 µL | 0.5 µL | 0.5 µL | - |
| NcoI | - | - | - | - | - | - | - | - | - | - | - |
| EcoRI (b) | - | - | - | - | - | - | - | - | - | - | - |

EcoRI (a) assay date 2/05
EcoRI (b) assay date 7/05

Reactions were incubated in a waterbath at 37 °C for 3 hours.

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Lab Book Ref

JRH4712-63 (1)
JR4712-64 (2)
JR4712-66 (1)
jrh4712-76 (1)
jrh4712-77 (1)
jrh4712-78 (1)
jrh4712-80 (1)
jrh4712-81 (1)
jrh4712-83 (1)
jrh4712-84 (1)
jrh4712-85 (1)
jrh4712-86 (1)
jrh4712-87 (1)
jrh4712-88 (1)
jrh4712-89 (1)
jrh4712-90 (1)

Product
jrh4712-74 (1)
jrh4712-76 (1)
jrh4712-76a (1)

Mutagenesis of plasmid p042 via Taq and Genemorph

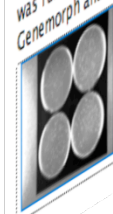
9th January 2007 @ 14:34

Lab Book Ref: jrh4712-78

Mutagenic PCR reactions were set up according to the following:

| | Taq | Genemorph | +ve ctrl | -ve ctrl |
|--------------------|---------|-----------|----------|----------|
| p042 | 2.5 µL | 1 µL | 20.5 µL | 0 µL |
| Water | 10 µL | 38 µL | 10 µL | 25.5 µL |
| 5 x GoTaq buffer | - | 5 µL | 5 µL | 5 µL |
| mutazyme buffer | - | - | - | - |
| Ordinary dNTPs | 5 µL | 1 µL | 3.5 µL | 3.5 µL |
| mutagenic dNTP mix | - | - | - | - |
| Mutazyme dNTP mix | 2.5 µL | - | 2.5 µL | 2.5 µL |
| MgCl2 | 12.5 µL | 2 µL | 2.5 µL | 2.5 µL |
| MnCl2 | 2.5 µL | 2 µL | 2.5 µL | 2.5 µL |
| Primer fwd | 2.5 µL | 2 µL | 1 µL | 1 µL |
| Primer rev | 1 µL | - | - | - |
| GoTaq | - | 1 µL | - | - |
| Mutazyme | - | - | - | - |

*GoTaq=1 µL stock + 3 µL water.
The reactions were run on program MUTAGBC for 30 cycles. 5 µL product was run on a 1% normal agarose analytical gel. Taq mutagenesis had failed, Genemorph and +ve ctrl had worked. -ve control was correct.



Jennifer Hale | [Beta-glucuronidase](#) | Comments (3)

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LabTrove: Easy Communication

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

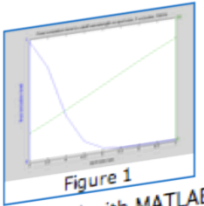


Figure 1

Published with MATLAB® 7.11.1

/Volumes/ifs/PhysicsAstronomyResearch/Private/xraylab/grants/2012 OPO HHG

Comments (0)

William Brocklesby | View Source

Computational processes also blog

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

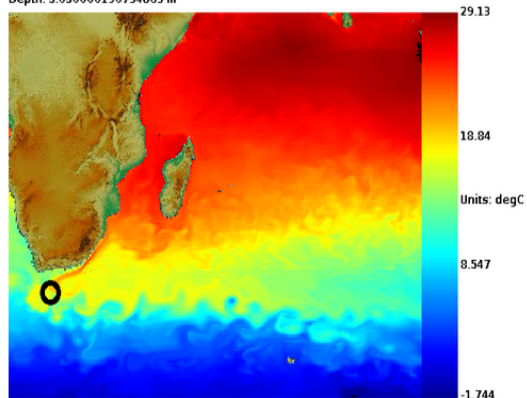
Elevationunits: m

Elevationpositive: down

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

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

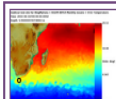
Depth: 5.050000190734863 m



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.

Attached Files



This Post

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[M \(13\)](#)

Elevationpositive

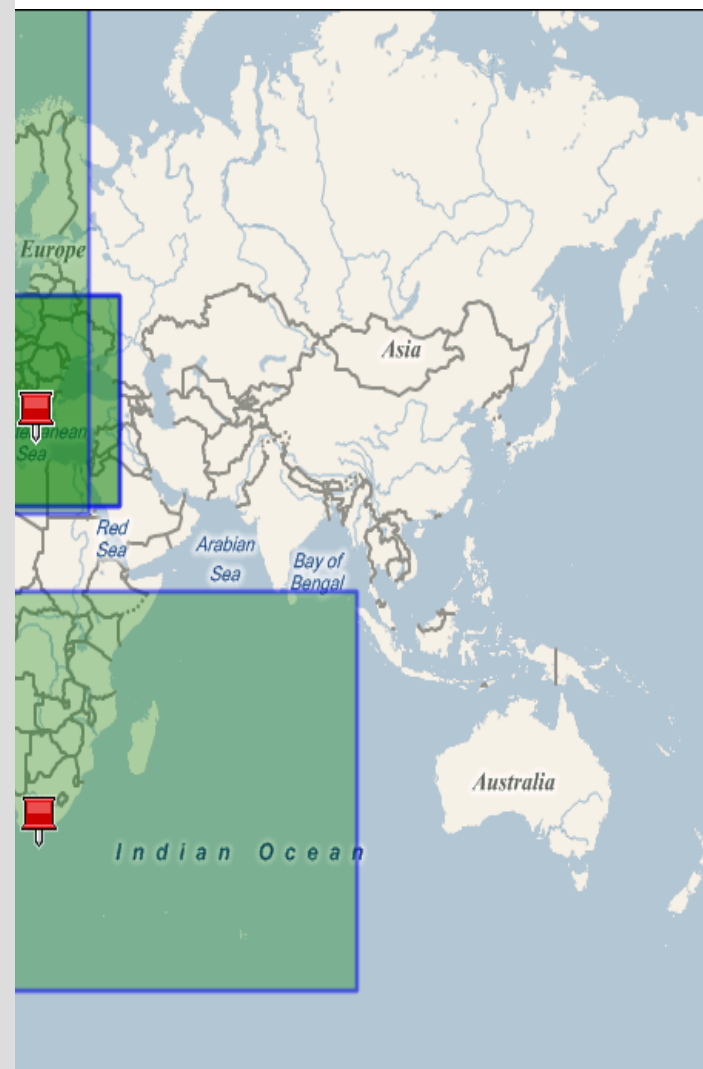
[Down \(13\)](#)

Tools

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BlogMyData Project - Godiva



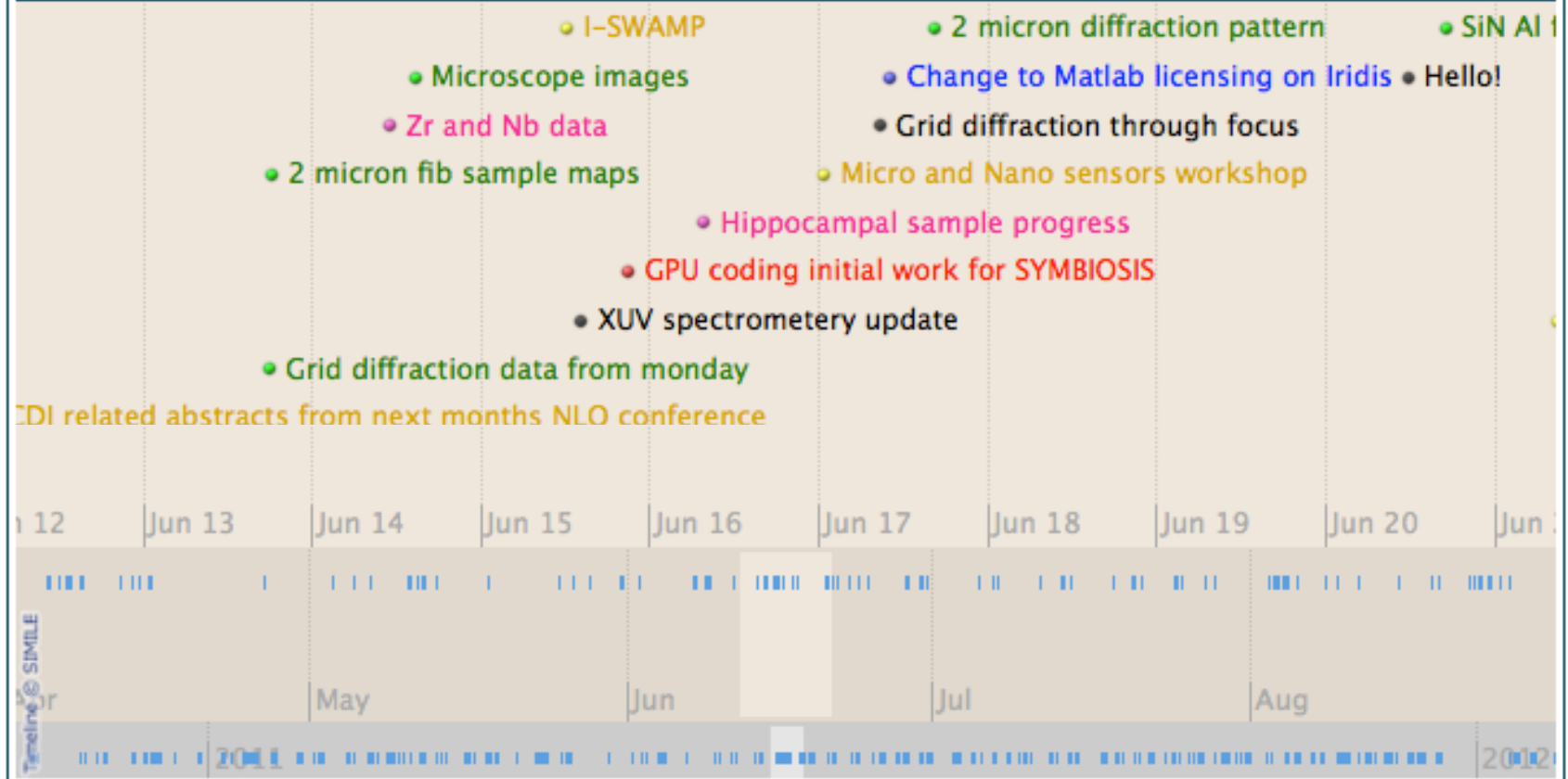
UltraFast Xray Group

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Search

Timeline



LabTrove Open Notebooks Mat Todd's PZQ Project

Praziquantel – Open Science

Praziquantel Project

- Introduction
- Project Updates
- Project Discussion
- ALTC links

Student Collaboration

- Hydrolysis of PZQ
- Resolution of PZQ
- Synthesis of Resolving Agents
- Conversion of PZQamine to PZQ

Example Blogs

- Pictet-Spengler route to Praziquantel
- Racemic Resolution of Praziquantel and Praziquanamine
- Racemization of PZQamine

Powered by labtrove 2.2 © University of Southampton

Pictet-Spengler route to Praziquantel

Synthesis of SC2-1

16th August 2012 @ 10:38

Sc 1-30

Synthesis of SC2-1 from tryptamine and 4-nitrobenzaldehyde.

HKAC

RTS-1 and RTS-1 (3000-40)

Procedure followed

Archives

- August 2012 (34)
- July 2012 (20)
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- Experiments (256)
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Racemization of PZQ and PZQamine

Racemization of the resolving 5-(1-1-PZQamine) obtained from racemic resolution of rac-PZQamine

Repetition: Racemization of (S)-PZQamine (MW50-13) with Rh/C

13th April 2011 @ 08:07

Repetition of the racemization experiments on enantiomerized (S)-(+)-PZQamine with Rhodium on charcoal to verify the results.

Chemical reaction scheme showing the racemization of (S)-PZQamine to (R)-PZQamine using Rh/C in toluene.

See also: Racemization of 5-(1-1-PZQamine) with Pd/C (MW50-13 to MW10-13)

Archives

- April 2011 (6)
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Tools

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Racemic Resolution of Praziquantel and Praziquanamine

Separation of the enantiomers of Praziquantel and derivatives by racemic resolution

N-benzoyl protection of MNR7-6 to give MNR14-6

2nd August 2012 @ 09:06

Chemical reaction scheme showing the N-benzoyl protection of MNR7-6 to give MNR14-6 using TEA in DCM at 0°C to RT.

Hazard and Risk Assessment:

Procedure

To a cooled solution of MNR7-6 (7.3 g, 35.11 mmol) in DCM (170 mL) at 0°C was added triethylamine (7.34 mL, 52.66 mmol) and benzoyl chloride (4.48 mL, 36.62 mmol). The solution was stirred for 14 hours at room temperature. In the morning, the reaction was quenched with water (16L) and stirred for 30 minutes then the

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Sections

Praziquantel – Open Science

Hydrolysis of PZQ

Hydrolysis of PZQ – WCPZQ101

17th June 2011 @ 09:32

Preliminary step in procuring enantiopure PZQ: acid hydrolysis of rac-PZQ into rac-PZQamine.

See also: Hydrolysis of PZQ – Standard Conditions (KH-PZQ-1001); Hydrolysis of rac-PZQ (3040-13); Hydrolysis of rac-PZQ (3040-14); Optimizing the acid cleavage conditions it

Chemical reaction scheme showing the hydrolysis of rac-PZQ to rac-PZQamine using 1 N HCl in EtOH, reflux.

Procedure:

rac-PZQ (4.0 g, 12.8 mmol, 90% 312-5) was dissolved in a mixture of EtOH (30 mL) and 2N HCl

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Tools

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Praziquantel – Open Science

Introduction

About the project

17th February 2011 @ 21:51

"This page lists the blogs associated with a worldwide student-led research project – to optimize the preparation of enantiopure praziquantel. A description of how you can get involved is given in the PDF attached.

You can read the paper about this research project that's currently being assembled – it's not finished, but has a fair amount of primary information for background reading.

http://openwetware.org/wiki/Todd_PZQ_Resolution

You can also read a couple of recent updates Mat Todd gave on the coordination site, The Synthetic Leap (TSL). You can sign up to be a member of TSL, and to receive more updates.

<http://www.thissyntheticleap.org/node/338>
<http://www.thissyntheticleap.org/node/339>
<http://www.thissyntheticleap.org/node/331>

Feel free to browse a few pages on TSL, since there's quite a bit there.

Background to the whole idea behind the project is here:

<http://www.makem.com/news/2010/1/10/2010/1/fall/news/2010/50.html>
<http://www.makem.com/news/2010/1/10/2010/1/fall/news/2010/50.html>
<http://www.makem.com/news/2010/1/10/2010/1/fall/news/2010/50.html>

You can watch Mat Todd talk about what open science is, and how it relates to PZQ, here:

Archives

- February 2011 (1)

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Praziquantel – Open Science

Pictet-Spengler route to Praziquantel

Racemization of PZQ and PZQamine

Racemic Resolution of Praziquantel and

Hydrolysis of PZQ

Introduction

Praziquantel – Open Science

Improved Synthesis of an Important Drug via Student Collaboration

Praziquantel Project

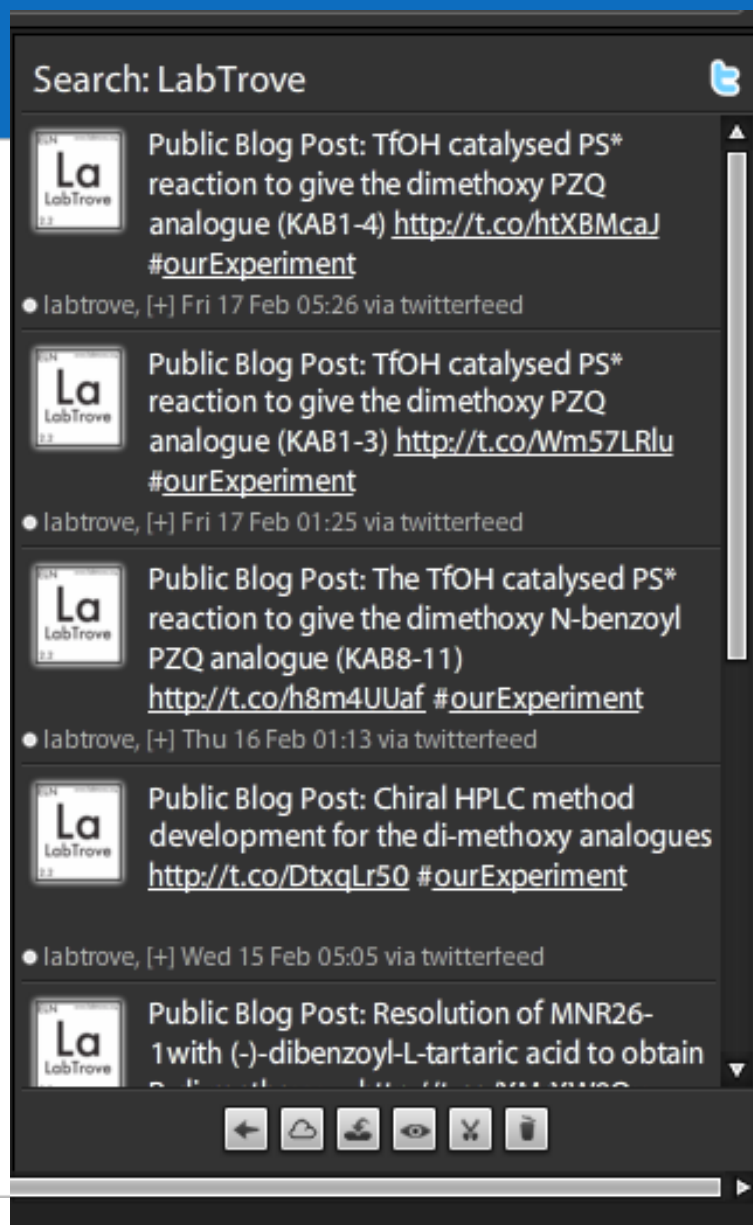
- [Introduction](#)
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Student Collaboration

- [Hydrolysis of PZQ](#)
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- [Conversion of PZQamine to PZQ](#)

Example Blogs

- [Pictet-Spengler route to Praziquantel](#)
- [Racemic Resolution of Praziquantel and Praziquanamine](#)
- [Racemization of PZQamine](#)

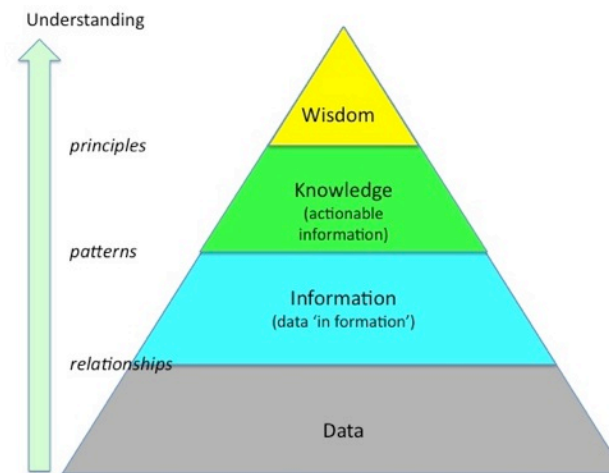


Open Notebooks

- Troves can be open Read/Comment/Write
 - Can control this access so it is your choice
- All contributions attributable (login needed)
 - Anonymous contributions not usually enabled
- Open contribution does worry the IT services
 - Provides potential pathway for abuse of systems
 - Not just our systems

Global open scientific notebook infrastructure

- Global collaboration:
 - International
 - Interdisciplinary
- Open science



- To ascend the *knowledge pyramid*, we need open collaboration and sharing of results

We must speed up the knowledge discovery process



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From The New Yorker Book of Technology Cartoons.

*All I am saying is that now is the time to
develop the technology to deflect an asteroid*