

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_D4128
pic_ECO42_D44035
EC042_D44062
SIGA_ECO42_D44035



Digital Research Data Sharing and Management

December 2011

Science is
increasingly
interdisciplinary

The DataCite logo, featuring a stylized 'D' icon followed by 'CITE' in a bold, sans-serif font, with the tagline 'because good research needs good data' below it.

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[Home](#) > [Resources for digital curators](#) > [Policy and legal](#) > [Overview of funders' data policies](#)

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Briefing Papers

How-to Guides

Overview of funders' data policies

The coverage of funders' publication and data policies

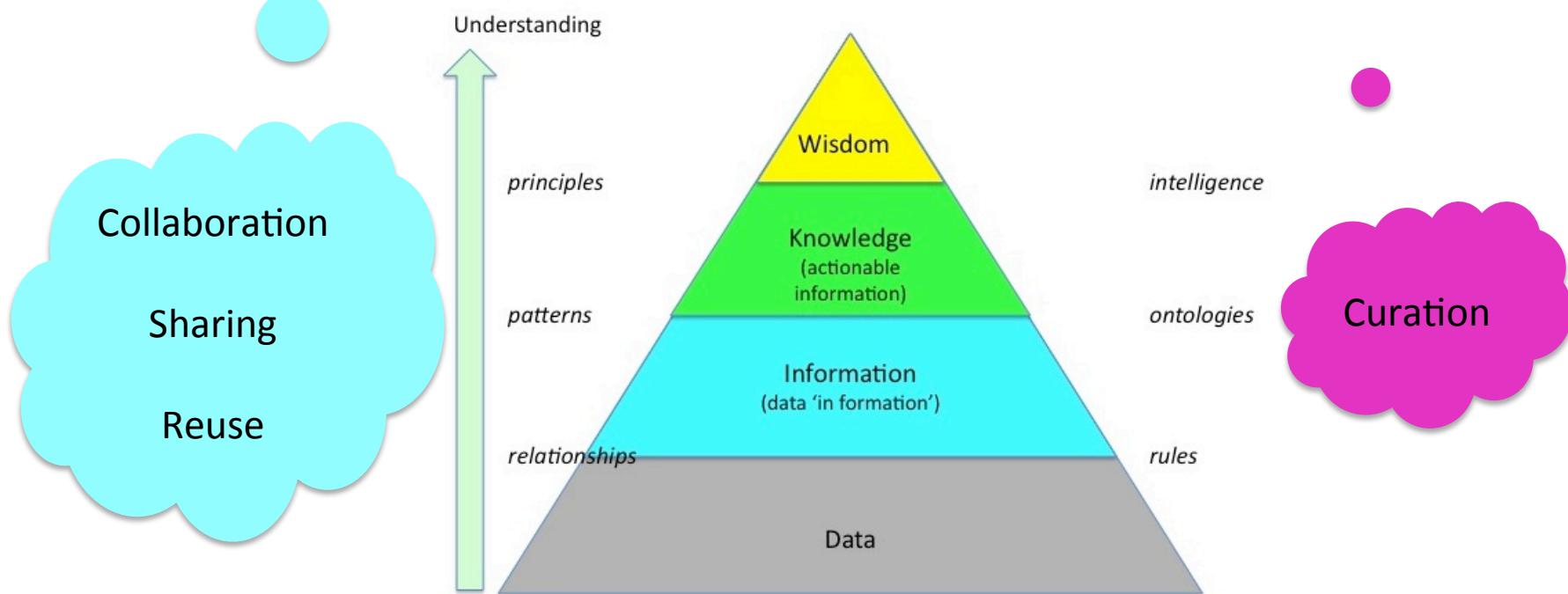
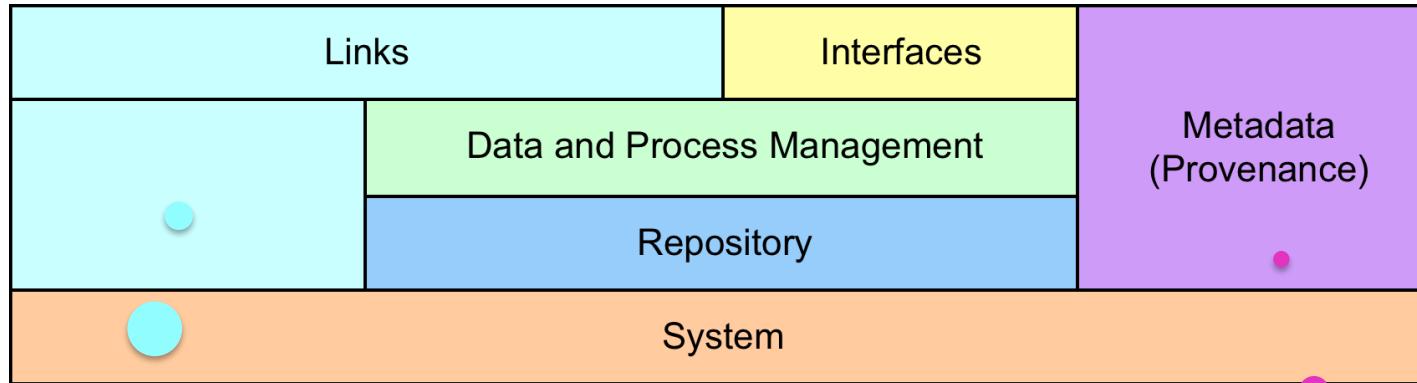


PRESS RELEASE

Brussels, 17 July 2012

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

Infrastructures - Architecture



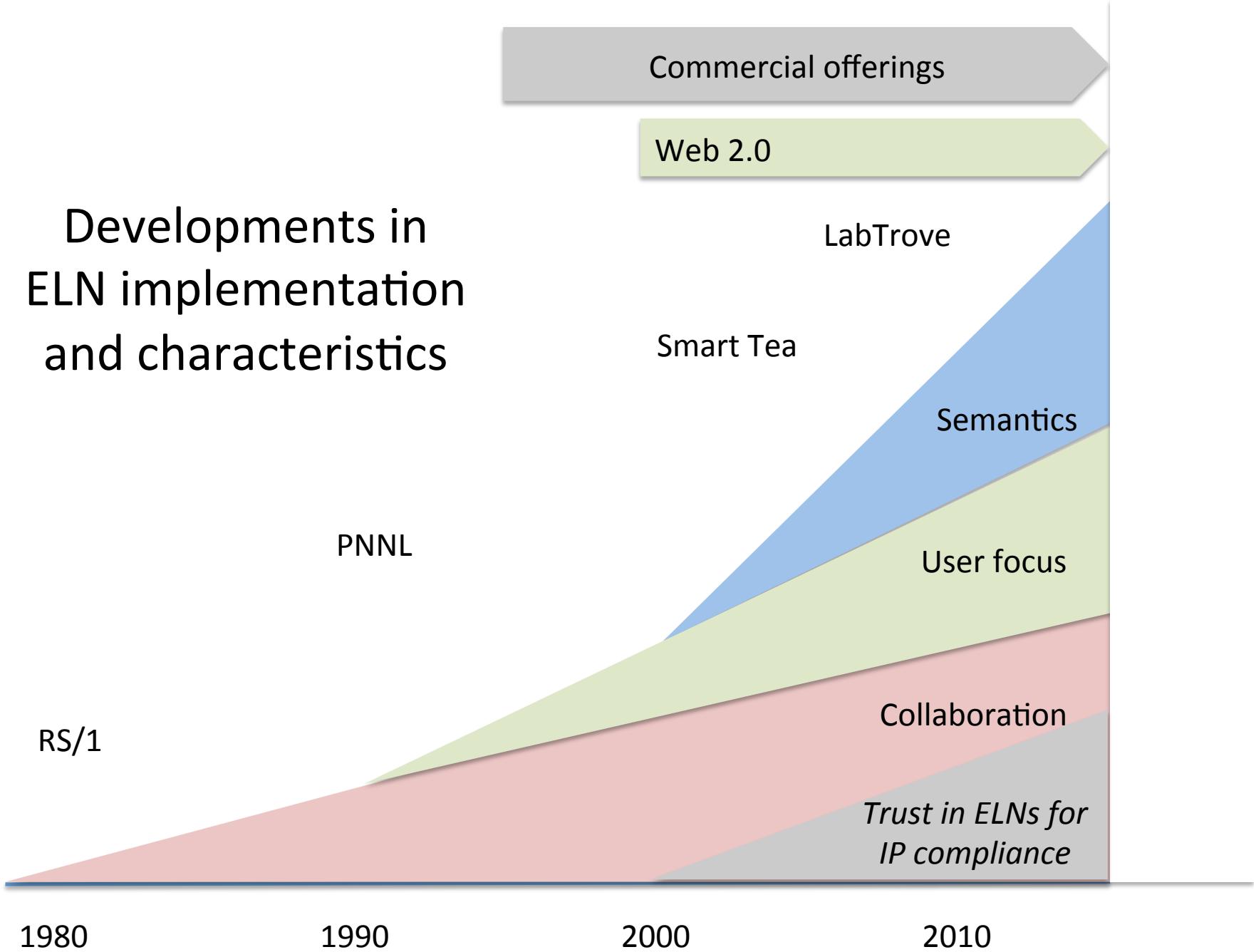
Comparison with
traditional paper
notebooks

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

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ourexperiment

Pictet-Spengler route to Praziquantel

Continuation: Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MW56-9 to MW56-12)

Continuation of Acid-catalyzed Pictet-Spengler reaction using methanesulfonic acid in various concentrations (MW56-8)

Continuation of Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MW56-5 to MW56-6)

Chemical reaction scheme: A bicyclic intermediate reacts with MeSO_3H under various conditions to form Praziquantel.

LabTrove enables the formation of a Smart Research

Older Posts >> Search

Archives

March 2011 (3)
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Tools

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LabTrove Public Blog Post: Synthesis of amine-linked analogue of TCMDC-123812 via reductive amination...
<http://t.co/BlashWbb> #malaria #drugdesign
yesterday · reply · retweet · favorite

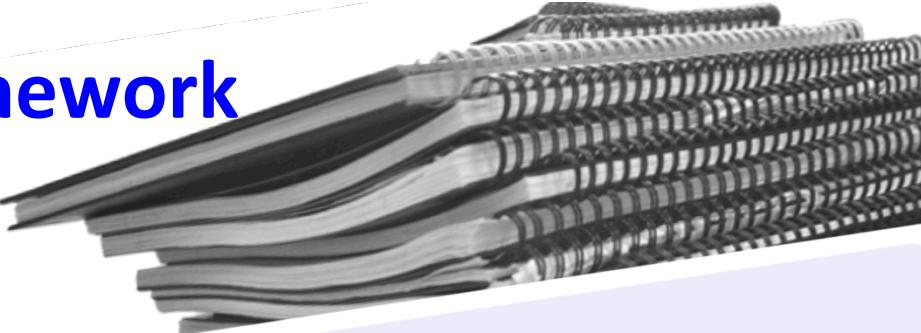
LabTrove Public Blog Post: Synthesis of ether-linked analogue of TCMDC-123812 (PMY 37-1) <http://t.co/XHqyRb8I> #malaria #drugdesign
yesterday · reply · retweet · favorite

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

<http://www.labtrove.org>

Smart Research Framework

My Lab Notebook



Introduction

The SRF project
a shared virtual
management.

Providing tools to meet the needs of responsibility, the use of projects, and mental a

LabTrove

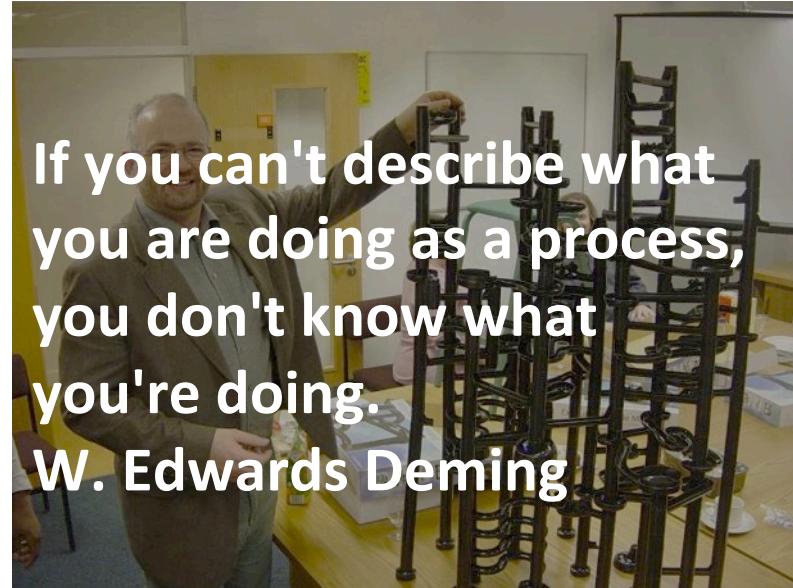
"preserving the record"



Introduction
Software Overview
Partners
Vision
SRF Software
LabTrove
plan3

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: Easy Communication



AutoTrove from Matlab

blogs@xray

WSB Matlab Autoblog

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

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This Blog

New Post

Timeline View

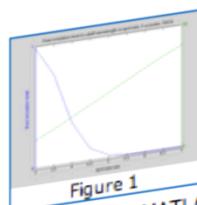
ion_vs_spot.m

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);
xlabel('spot size /um')
ylabel('final ionization level');
title(sprintf('Final ionization level & cutoff wavelength vs spot size, %g uJ pulse'))
%grid on
```



Published with MATLAB® 7.11.1

/Volumes/jfDfsResPhysicsAstronomyResearch\$/Private/xraylab/grants/2012 OPO HHG
Attached files
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Computational processes also blog
William Brocklesby | View Source Matlab Autoblog

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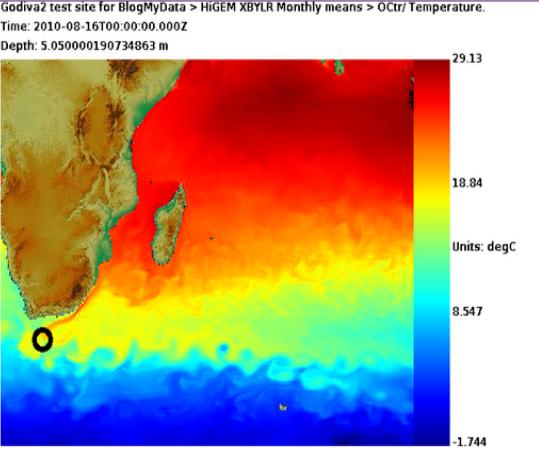
BlogMyData

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: OCtr/ 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 > OCtr/ Temperature.
Time: 2010-08-16T00:00:00.000Z
Depth: 5.050000190734863 m



Testing POI works

Search

This Post
Permalink
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Export:
XML (With Files)
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HiGEM_XBYLR_MONTHLYMEAN (13)

Variablestandardname
OCtr/ Temperature. (6)
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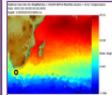
Calendarsystem
360 Day (13)

Elevationunits
M (13)

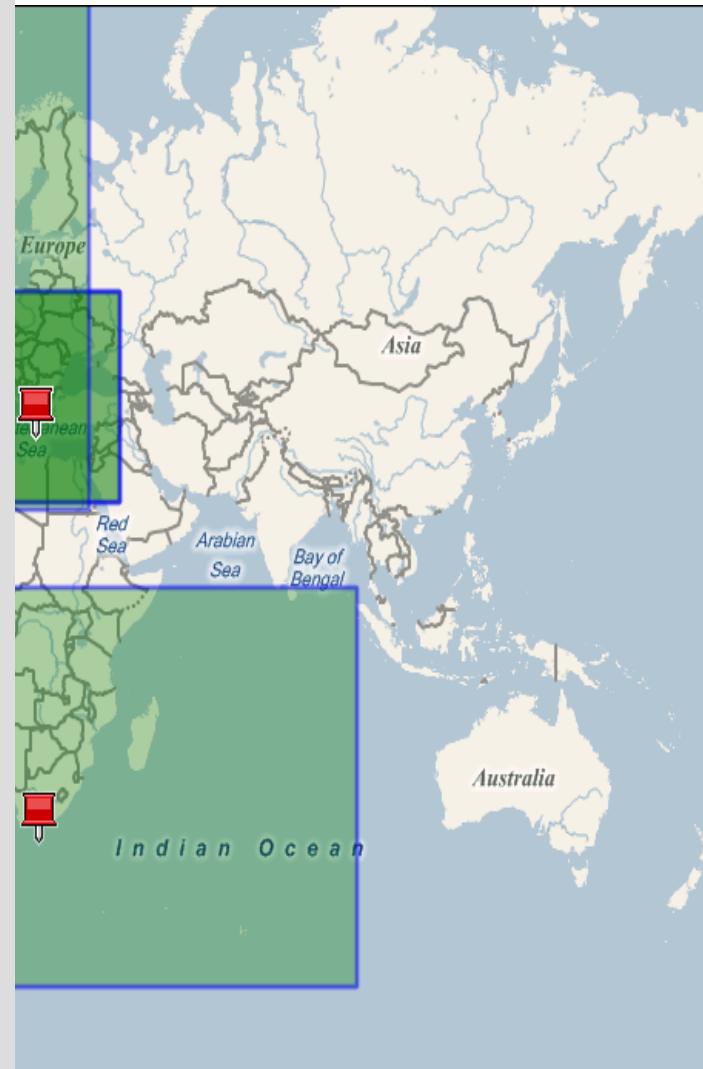
Elevationpositive
Down (13)

Tools
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Attached Files



BlogMyData Project - Godiva



UltraFast Xray Group

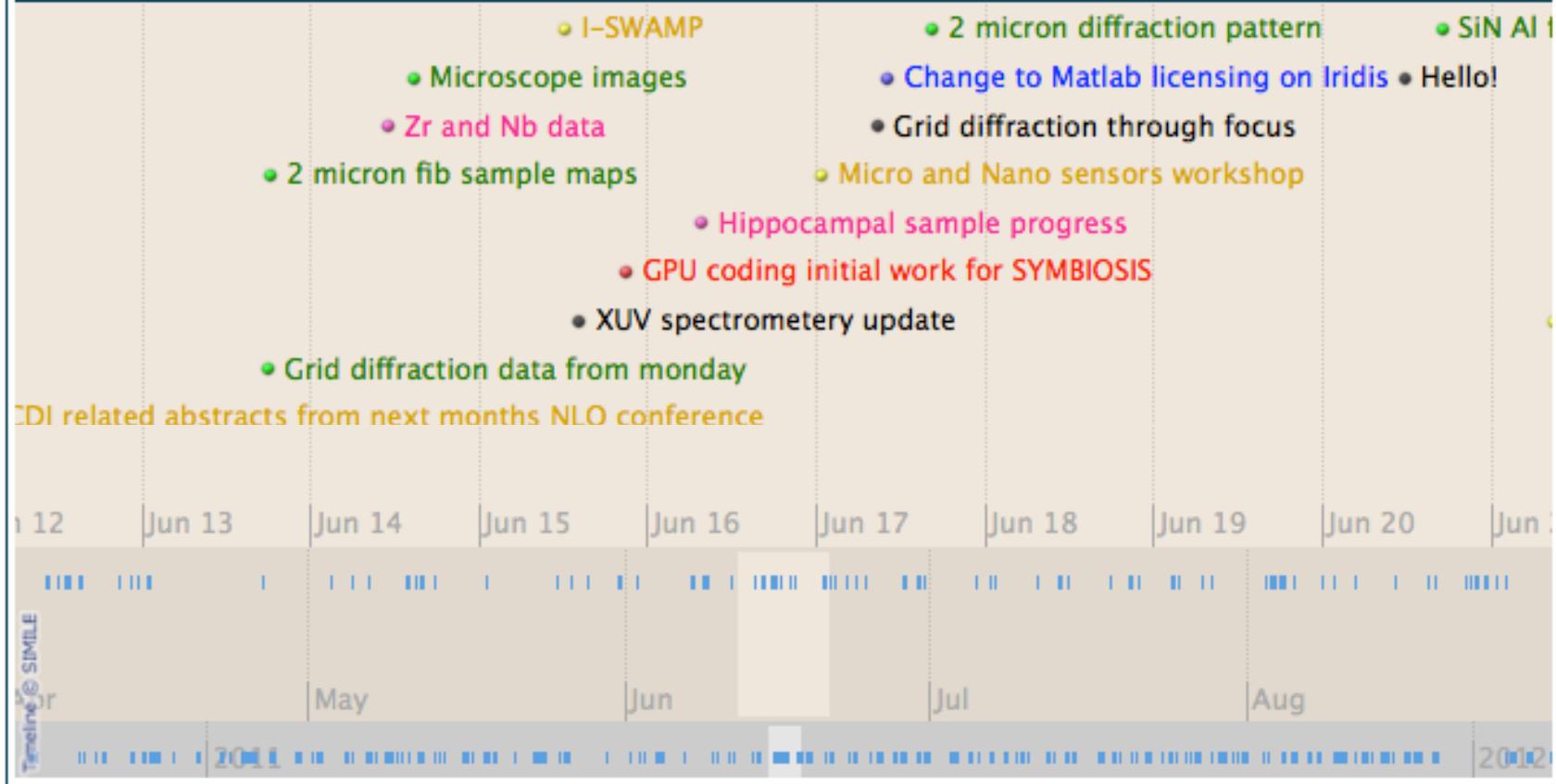
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Timeline



LabTrove Open Notebooks Mat Todd's PZQ Project

PZQ

Praziquantel – Open Science
Methods of an Open-Source Drug via Student Collaboration

Praziquantel Project

- Introduction
- Project Updates
- Project Overview
- ALTC Info

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 PZQ and PZQamine

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Praziquantel – Open Science

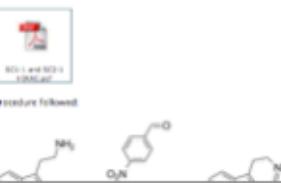
ourexperiment alpha

Pictet-Spengler route to Praziquantel
Synthesis of intermediates and derivatives of PZQ

Synthesis of SC2-1
18th August 2012 @ 03:38

Sc 1-10
Synthesis of SC2-1 from tryptamine and 4-nitrobenzaldehyde.

Procedure followed:



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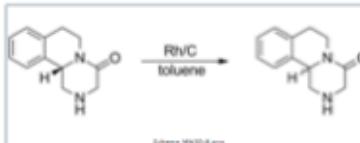
Pictet-Spengler route to Praziquantel

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Racemization of PZQ and PZQamine
Racemization of the enantiomeric S-(+)-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 enantioenriched (S)-(+)-PZQamine with Rhodium on charcoal to verify the results



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April 2011 (6)
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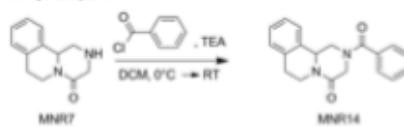
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Racemization of PZQ and PZQamine

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Racemic Resolution of Praziquantel and Praziquanamine
Resolution of the intermediates of Praziquantel and derivatives via racemic resolution

N-benzoyl protection of MNR7-6 to give MNR14-6
2nd August 2012 @ 03:06



Procedure

To a cooled solution of MNR7-6 (7.3 g, 35.13 mmol) in DCM (170 mL) at 0°C was added triethylamine (7.34 mL, 52.46 mmol) and benzoyl chloride (4.48 mL, 38.62 mmol). The solution was stirred for 14 hours at room temperature.

In the morning, the reaction was quenched with water (100 mL) and stirred for 30 minutes then the

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September 2010 (5)

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Racemic Resolution of Praziquantel and

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Praziquantel – Open Science

Hydrolysis of PZQ

Hydrolysis of PZQ – WCPZQ101
27th June 2011 @ 03:32

Preliminary step: In-proceeding enantioseparation PZQ, acid hydrolysis of rac-PZQ into rac-PZQamine.

See also:

Hydrolysis of PZQ – Standard Conditions (68-PZQ-1001)
Hydrolysis of rac-PZQ (94-PZQ-13)
Hydrolysis of rac-PZQ (94-PZQ-14)
Optimizing the acid and cleavage conditions: II



Procedure

rac-PZQ (4.0 g, 12.8 mmol, MW: 312.5) was dissolved in a mixture of EtOH (30 mL) and 2N HCl

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Hydrolysis of PZQ

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Introduction

About the project
17th February 2011 @ 01:53

This page lists the blogs associated with a worldwide student-led research project – to optimize the production of enantiomeric 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://opennotebook.org/wiki/Todd_PZQ_Resolution

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

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

Please free to browse a few pages on TL, since there's quite a bit there.

Background to the whole idea behind this project is here:

<http://www.nature.com/news/2010/100294/full/news.2010.30.html>
http://www.ncbi.nlm.nih.gov/pmc/articles/PMC287022/pdf/2010/CA_jun07p2.pdf (this is a pdf file)

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

Introduction

Praziquantel – Open Science

Improved Synthesis of an Important Drug via Student Collaboration

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](#)

Search: LabTrove 

Public Blog Post: TfOH catalysed PS* reaction to give the dimethoxy PZQ analogue (KAB1-4) <http://t.co/htXBMcaJ> #ourExperiment

• labtrove, [+] Fri 17 Feb 05:26 via twitterfeed

Public Blog Post: TfOH catalysed PS* reaction to give the dimethoxy PZQ analogue (KAB1-3) <http://t.co/Wm57LRlu> #ourExperiment

• labtrove, [+] Fri 17 Feb 01:25 via twitterfeed

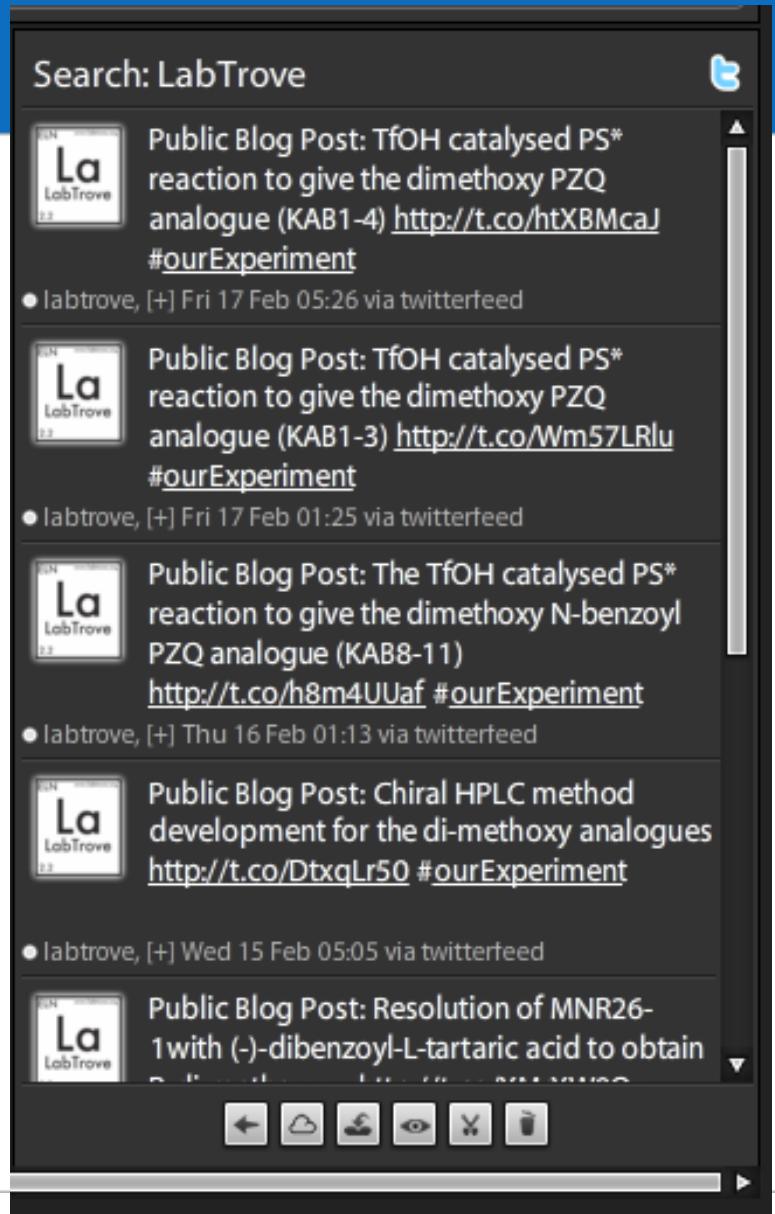
Public Blog Post: The TfOH catalysed PS* reaction to give the dimethoxy N-benzoyl PZQ analogue (KAB8-11) <http://t.co/h8m4UUaf> #ourExperiment

• labtrove, [+] Thu 16 Feb 01:13 via twitterfeed

Public Blog Post: Chiral HPLC method development for the di-methoxy analogues <http://t.co/DtxqLr50> #ourExperiment

• labtrove, [+] Wed 15 Feb 05:05 via twitterfeed

Public Blog Post: Resolution of MNR26-1 with (-)-dibenzoyl-L-tartaric acid to obtain

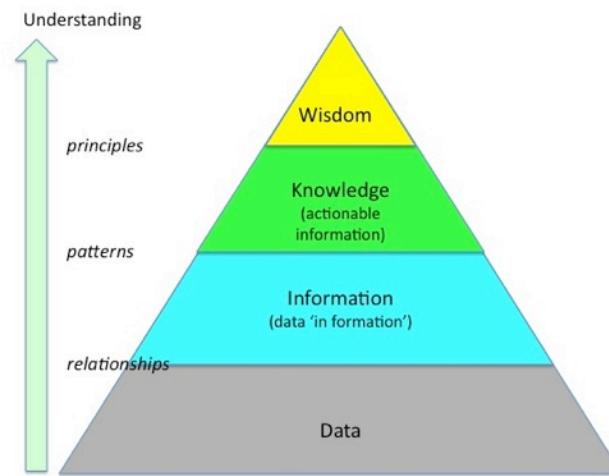


Open Notebooks

- 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*