

DEVELOPING AN OPEN SOURCE ELN TO SUPPORT OPEN & INTERDISCIPLINARY SCIENCE

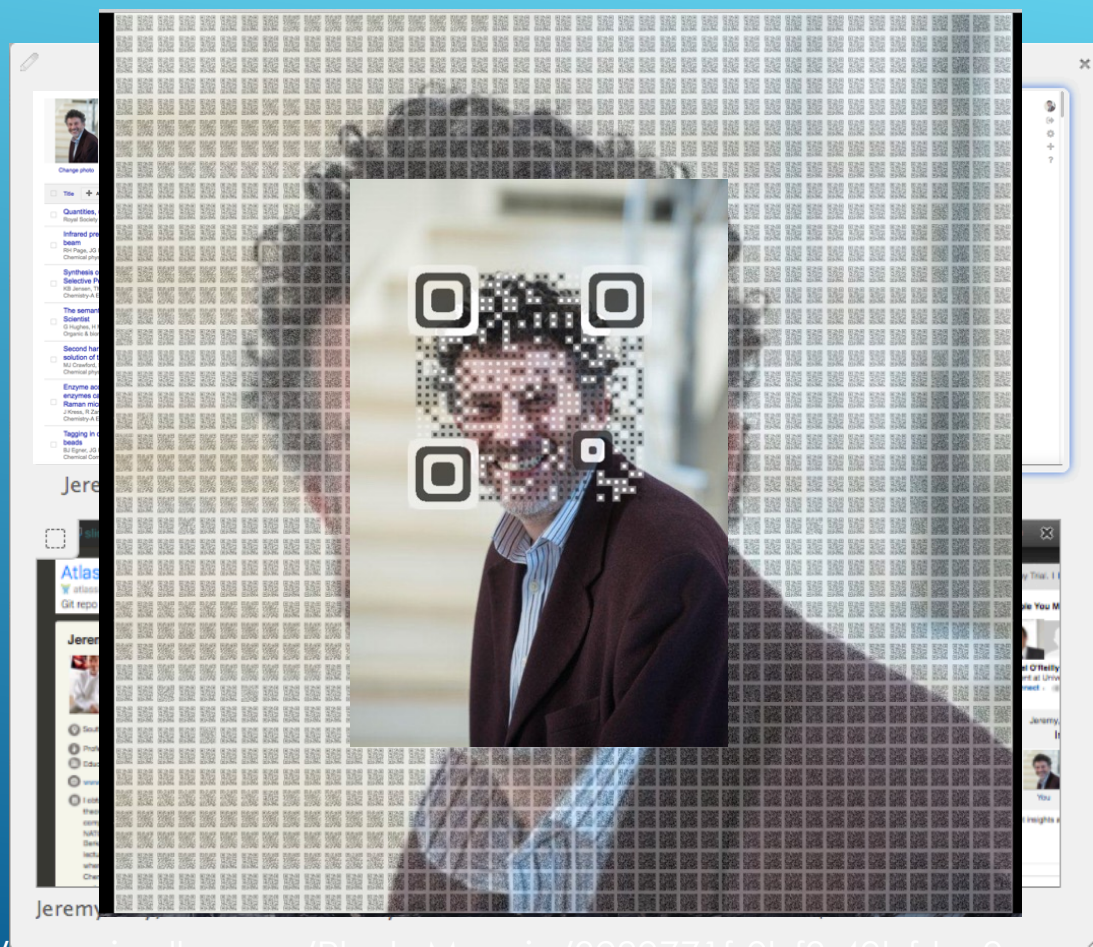
Jeremy G. Frey

University of Southampton

@profechem

Jeremy Frey LabTrove ELN

A Chemist's Digital Aura



Jeremy Frey LabTrove ELN

<http://mosaicdaily.com/PhotoMosaic/328977/1f-0b13-49b1-bc8d-181017004ff>

2

13/01/2017

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Chemists escape labs via mobiles

By Jo Twist
BBC News science and technology reporter

A blend of mobile technology and award-winning software is letting scientists finally escape the lab.

The software, called "middleware", lets different computer systems talk to each other securely and instantaneously.

As part of a national e-Science project in the UK, it is being used to let Southampton University chemists monitor experiment conditions from mobiles.

Sensors in the lab pick up any changes in the environment so the system can alert chemists, wherever they are.

"It replaces the traditional notebook with some electronic form

The system is not smart enough to actually buy a round yet

Past, Present and Future

Research Notetaking in the Digital Era



Jeremy Frey LabTrove ELN

The three Norns (Fates)

Cite this: Chem. Soc. Rev., 2013, 42, 8157

Received 30th March 2013
DOI: 10.1039/c3cs00122f

www.rsc.org/csr

Laboratory notebooks in the digital era: the role of ELNs in record keeping for chemistry and other sciences

Colin L. Bird, Cerys Willoughby and Jeremy G. Frey*

Egyptian evidence of scientific records dates back almost 50 centuries. In more recent times da Vinci and Faraday provide role models for scrupulous recording of ideas, observations, and conclusions. Their medium was paper, but despite the quality of their notebooks, we cannot turn the clock back. Our primary purpose is to review the influences of the digital era on scientific record keeping. We examine the foundations of the emerging opportunities for preserving and curating electronic records focussing on electronic laboratory notebooks (ELNs), with an emphasis on their characteristics and usability.

Introduction

The origin of science itself is a subject for philosophical discussion; so dating the first recording of a scientific endeavour must almost inevitably also be a matter for speculation. However, we do know of an instance of recorded occupational medicine that has been attributed to the Egyptian architect,

physician, and statesman Imhotep (27th century BCE), based on a study of the Edwin Smith papyrus.¹

The History of Science article in Wikipedia covers the development of science and scientific methodology from the ancient civilisations through to the modern era, and includes several examples of the recording of information in a manner that we could regard as scientific. Observations were represented numerically as well as in narrative form, for example the recording of astronomical information in Mesopotamia.² There is also historical evidence of the reuse and repurposing of

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Colin L. Bird

Having obtained his BSc and PhD in Chemistry at the University of Southampton, Colin Bird joined IBM UK Laboratories. After contributing to IBM's electrochromic display technology he transferred to the IBM UK Scientific Centre to develop advanced image and visualisation applications. His work on content-based image retrieval led to a one-year secondment in 1999 back to the University of Southampton. On returning to IBM, he was involved in various aspects of information management, specialising in classification and metadata, and became an information architect. When he left IBM, he resumed his collaboration with Professor Jeremy Frey on e-Research projects, which began in 2000 as an industrial partner for the CombeChem project.



Cerys Willoughby

Cerys Willoughby obtained her BSc in Geology from the University of Wales, Aberystwyth and her MSc in Environmental Sciences from University of Wales, Swansea. After spending some time teaching teenagers and adults, she joined IBM UK Laboratories as a software engineer. Working in a variety of roles in the company she specialised in usability and information architecture. She began collaborating with Professor Jeremy Frey in 2007 as a guest lecturer on usability and accessibility for an e-Research course and is currently undertaking a part-time PhD at the University of Southampton.

COLIN L. BIRD, CERYS WILLOUGHBY,
SIMON J. COLES, & JEREMY G. FREY

DATA CURATION

ISSUES IN THE CHEMICAL SCIENCES

All science is strongly dependent on preserving, maintaining, and adding value to the research record, including the data, both raw and derived, generated during the scientific process. This statement leads naturally to the assertion that all science is strongly dependent on curation.^[1]

Chemistry is no exception, and given the significance of chemical data to many other disciplines, we assert that curation should be a fundamental aspect of the research practice in the chemical sciences. In this article we investigate the extent to which chemists do actually respect the importance of curation in their day-to-day activities in the laboratory or, nowadays, frequently at the computer. »



Cite this: Chem. Sci., 2013, 4, 1614

Received 17th July 2014
Accepted 20th October 2014

DOI: 10.1039/c4cs00228b

www.rsc.org/chemicalscience

Experiences with a researcher-centric ELN†

Katrina A. Badiola,^a Colin Bird,^b William S. Brocklesby,^c John Casson,^d Richard T. Chapman,^e Simon J. Coles,^b James R. Cronshaw,^a Adam Fisher,^b Jeremy G. Frey,^{b,f} Danmar Gloria,^g Martin C. Grosse,^h D. Brynn Hibbert,ⁱ Nicola Knight,^j Lucy K. Mapp,^j Luke Marazzi,^j Brian Matthews,^j Andy Milsted,^h Russell S. Minns,^j Karl T. Muelier,^j Kelly Murphy,^j Tim Parkinson,^j Rosanne Quinnell,^a John S. Robinson,^h Murray N. Robertson,^j Michael Robins,^j Emma Springate,^g Graham Tizzard,^g Matthew H. Todd,^a Alice E. Williamson,^g Cerys Willoughby,^b Erica Yang^g and Paul M. Ylloja^a

Electronic Laboratory Notebooks (ELNs) are progressively replacing traditional paper books in both commercial research establishments and academic institutions. University researchers require specific features from ELNs, given the need to promote cross-institutional collaborative working, to enable the sharing of procedures and results, and to facilitate publication. The LabTrove ELN, which we use as our exemplar, was designed to be researcher-centric (i.e., not only aimed at the individual researcher's basic needs rather than to a specific institutional or subject or disciplinary agenda, but also able to be tailored because it is open source). LabTrove is being used in a heterogeneous set of academic laboratories, for a range of purposes, including analytical chemistry, X-ray studies, drug discovery and a biomaterials project. Researchers use the ELN for recording experiments, preserving data collected, and for project coordination. This perspective article describes the experiences of those researchers from several viewpoints, demonstrating how a web-based open source electronic notebook can meet the diverse needs of academic researchers.

1 Introduction

Electronic Laboratory Notebooks (ELNs) are progressively replacing traditional paper books for keeping the experimental record,¹ especially in commercial research establishments. Important drivers for this change are the need to comply with regulatory requirements and the desire to protect and expand intellectual property (IP); structured notebook systems should provide the necessary audit trails.² ELNs offer considerably more to researchers and to research groups than do systems

that offer only content management and sharing facilities. ELNs unite the objects that comprise the record of research and preserve the provenance of each object and its contribution to the overall narrative.

The 2013 review of laboratory notebooks in the digital era (by three of the authors)³ not only explores the history and the expanding use of electronic laboratory notebooks but also presents the results of a comprehensive survey of the literature relating to ELNs. It is clear from the survey and from considerations of the scientific applications for which ELNs have been deployed that digital notebooks come in a range of embodiments. The distinction between commercial and academic institutions is but one aspect; in many cases the designers of ELNs have adapted both the input and output to match the specific applications for which the ELNs are used. Most ELNs, especially the major commercial offerings, are proprietary. There is, however, increasing interest in open source implementations, as they enable individual laboratories or institutions to tailor the operation and the data preservation to suit their particular needs. The review also examines the social and technical issues that combine to influence moves from paper to digital notebooks.

There are many concerns in the academic environment with the adoption of digital notebooks. The obvious issues of cost are significant but more fundamental are the concerns with the

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ⁱElectronic supplementary information (ESI) available. See DOI: 10.1039/c4cs00228b

http://commons.wikimedia.org/wiki/File:ISS-30_Ice_floes_along_the_Kamchatka_coastline.jpg



Reducing and Managing Uncertainty

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Science as an open enterprise Final report

21 June 2012

The Science as an open enterprise report highlights the need to grapple with the huge deluge of data created by modern technologies in order to preserve the principle of openness and to exploit data in ways that have the potential to create a second open science revolution.

Exploring massive amounts of data using modern digital technologies has enormous potential for science and its application in public policy and business. The report maps out the changes that are required by scientists, their institutions and those that fund and support science if this potential is to be realised.

Areas for action

Six key areas for action are highlighted in the report:

- Scientists need to be more open among themselves and with the public and media
- Greater recognition needs to be given to the value of data gathering, analysis and communication
- Common standards for sharing information are required to make it widely usable

Download

Final report
PDF, 8.4 MB

Additional downloads

Summary
PDF, 4.7 MB

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ZIP, 4.7 MB

References (BibTeX)
ZIP, 8.1 KB

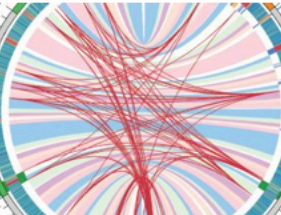
Science as an open enterprise

Final report, case studies of data use and data repositories and the launch event
published June 2012

Public meeting and seminar
held in November 2011

Call for evidence
closed August 2011

The Spanish Cucumber E. Coli. This genome was analysed within weeks of its outbreak because of a global and open effort; data about the strain's genome sequence were released freely over the internet as soon as they were produced.



Intelligent Open Access to Data

Jeremy Frey LabTrove ELN

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Page last updated at 14:56 GMT, Tuesday, 1 December 2009

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'Show Your Working': What 'ClimateGate' means

VIEWPOINT
Mike Hulme and Jerome Ravetz

The "ClimateGate" affair - the publication of e-mails and documents hacked or leaked from one of the world's leading

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A weekly series of thought-provoking opinion pieces on environmental topics
Reviving Rio

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The musings and ravings of a computational biologist about science, computers, music and, you know, stuff

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Structuregate?

December 10th, 2009

The University of Alabama at Birmingham issued a [statement](#) last week asking that 11 structures be removed from the Protein Data Bank, as they are quite possibly fabricated. Wow. Very little detail was given by UAB's statement (below), or by the media. Apparently all the structures are tied to one person, HMK Murthy, who could not be reached or traced, as reported by the Birmingham News.

The structures' PDB codes are:

1CMW, 1DF9/2QID, 1G40, 1G44, 1L6L, 20U1, 1R3D, 1Y8E, 2G7Y, 2G80. Some of these are still in the databank.

The University of Alabama at Birmingham has requested that the [Research Collaboratory for Structural Bioinformatics Protein Data Bank](#) remove certain protein structure files deposited by a former UAB employee. UAB also has identified nine publications related to the same protein structures that should be retracted from various scientific journals, and is making those journals aware of this matter.

Allegations of data fabrication and/or falsification were made concerning certain protein structures published by the former UAB employee. In accordance with UAB's scientific integrity policy, and that of the Office of Research Integrity of the U.S. Department of Health & Human Services, UAB empanelled a committee of experts with no conflicting interests to investigate these allegations. After a thorough examination of the available data, which included a re-analysis of each structure alleged to have

codehead.com...

StructureGate

13/01/2017

7342.pdf (6 pages)

Water surface is acidic

Victoria Buch^{*}, Anne Milet[†], Robert Vácha[‡], Pavel Junowirth[§], and J. Paul Devlin[¶]

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Featured Research

from universities, journals, and other organizations

Rewrite the textbooks on water's surface tension: Air-water interface is negatively charged by the adsorption of hydroxide ions

Date: March 19, 2014 Share This

Source: University of Melbourne

Summary: Researchers in Australia make significant difference in the water used by the next generation of biophysicists and engineers. The latest investigations have shown that the physical Chemistry of water is charged by the adsorption of hydroxide ions.

Related Topics

Matter & Energy

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- > Inorganic Chemistry
- > Thermodynamics
- > Biochemistry
- > Nuclear Energy

used in engineering. These long-standing chemical problems have been negatively affected by the adsorption of hydroxide ions. However, the high computational cost of the model system, the duration of the simulation was carried out for water with a pair of H_3O^+ and OH^- ions, the simulation was carried out for boundaries and a slab with two open boundaries. This "on-the-fly" technique modeling of proton transfer systems on transfer and transitions between different forms are automatically included in the model. However, the high computational cost of the model system, the duration of the simulation was carried out for water with a pair of H_3O^+ and OH^- ions, the simulation was carried out for boundaries and a slab with two open boundaries. This "on-the-fly" technique modeling of proton transfer systems on transfer and transitions between different forms are automatically included in the model.

December 19, 2006)

used. First, constant volume and molecular dynamics simulations of water with a pair of H_3O^+ and OH^- ions, the simulation was carried out for boundaries and a slab with two open boundaries. This "on-the-fly" technique modeling of proton transfer systems on transfer and transitions between different forms are automatically included in the model. However, the high computational cost of the model system, the duration of the simulation was carried out for water with a pair of H_3O^+ and OH^- ions, the simulation was carried out for boundaries and a slab with two open boundaries. This "on-the-fly" technique modeling of proton transfer systems on transfer and transitions between different forms are automatically included in the model.

PAPER www.rsc.org/faraday_d | Faraday Discussions

The surface of neat water is basic

James K. Beattie,^{*} Alex M. Djerdjev and Gregory G. Warr

Received 28th March 2008, Accepted 28th May 2008
First published as an Advance Article on the web 18th September 2008
DOI: 10.1039/b805266b



If only I knew exactly how she did this experiments

I wish I had recorded things at the start the way I do now.....

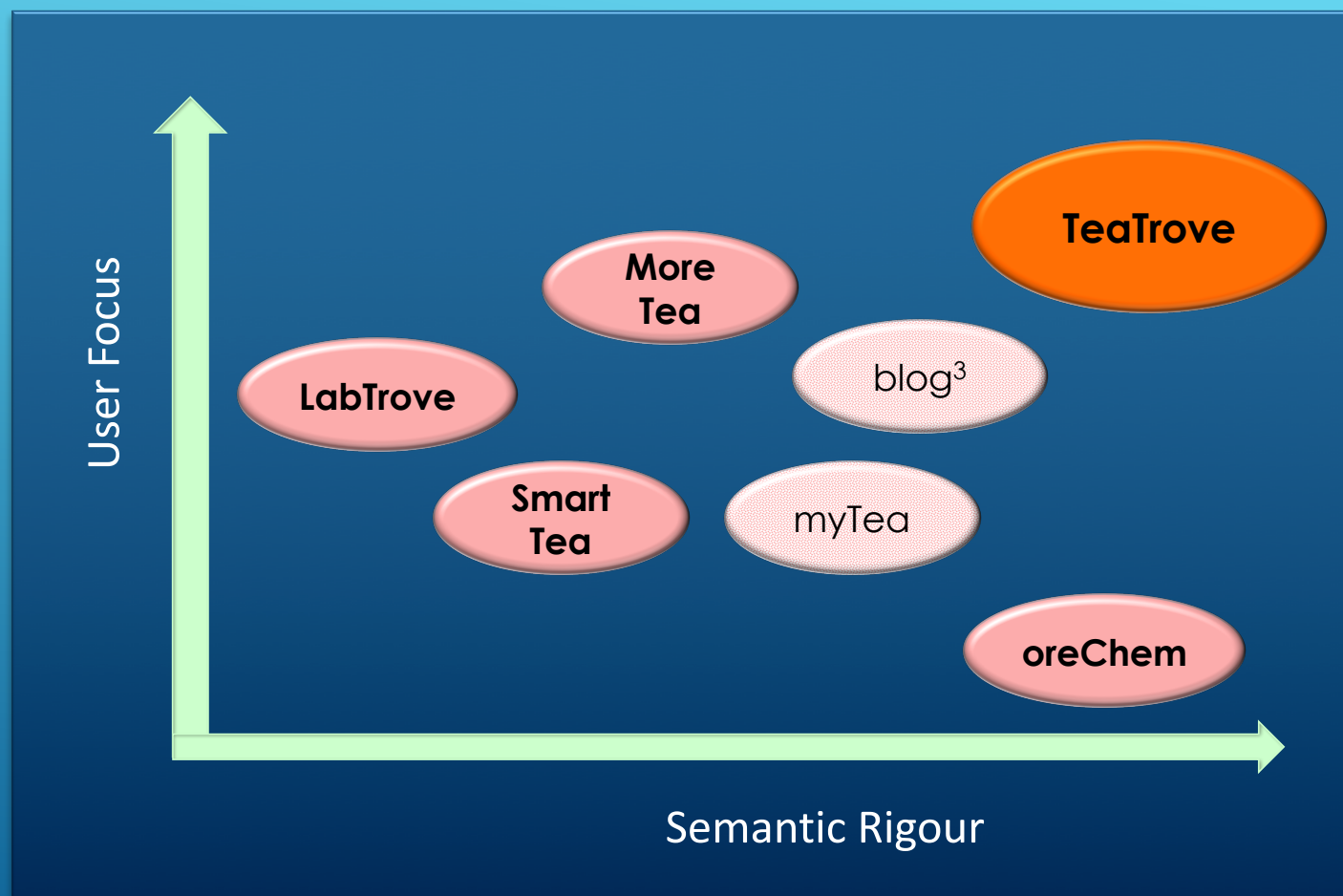
I know all this supplementary information could be useful but will people really remember the format? Is it worth all the hassle?

I wish I could get the numbers from this graph - the pdf is not much use.

Typical Laboratory



WHATS THE STORY IN BALAMORY,
WOULDN'T YOU LIKE TO KNOW?



The Trove Software

LabTrove

"preserving the record"

© flickr.com/julio_manzerova

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our experiment

Pictet-Spengler route to Praziquantel

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

Continuation of Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MSA-9 to MSA-12)

LabTrove enables the formation of a Smart Research

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labtrove Public Blog Post: Synthesis of amine-linked analogue of TCMDC-123812 via reductive amination...
<http://t.co/BiaShWbb> #malaria #drugdesign
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labtrove Public Blog Post: Synthesis of ether-linked analogue of TCMDC-123812 (PMY 37-1) <http://t.co/XhgyRb8I> #malaria #drugdesign
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labtrove Public Blog Post: Synthesis of 2-Ethoxycarbonylthiolan-3-one <http://t.co/m9mUBQKS> #malaria

www.labtrove.org

Jeremy Frey LabTrove ELN

12

13/01/2017

- ▶ LabTrove - E-Science and Jisc Funding
- ▶ Open Source Software – code available
- ▶ Hosted on Southampton servers or researchers own hardware
- ▶ Entries stored as ASCII XML, Files native format
- ▶ Support for basic research needs in a flexible way
- ▶ Allow researchers to use their own tools
- ▶ Export and Archive abilities
- ▶ Business Model and Community

OPEN SOURCE WEB BASED

New Entry

Font Siz

Downloaded from <http://ajph.org/> on November 10, 2015

Key



 Add sketch  Upload data

Transformation of plasmid JRH4712/66 into BW25141 by electroporation

11th December 2006 @ 14:31

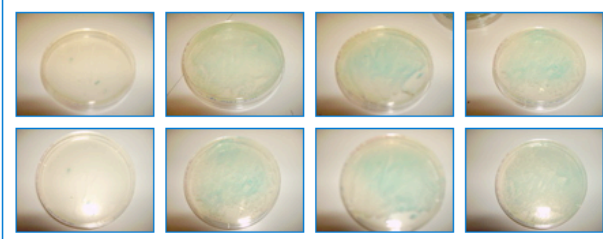
Transformations were set up according to the following protocol: LB Ampicillin arabinose plates and SOC medium were warmed to 37 °C briefly before the arabinose plates were spread with X-glu (80 µL, 1:1 X-glu and LB) and allowed to continue warming.

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 incubated at 37 °C for one hour with shaking. The transformants were diluted 1 in 20 with LB and 100 µL added to LB amp arabinose plates and incubated at 37 °C overnight.

Data



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

Archives

January 2007 (24)
December 2006 (11)
November 2006 (5)

Sections

[beta-galactosidase preparation and assays \(18\)](#)
[Beta-glucuronidase \(18\)](#)
[Data \(Formatting\) \(1\)](#)
[Software discussions \(2\)](#)
[Starting materials and reagents \(1\)](#)

Lab Book Ref

JRH4712-63 (1)
JR4712-64 (2)
JR4712-66 (1)

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 Parent2: jrh4712-80_white

Digestions were set up as follows:

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

EcoRI (a) assay date 2/05

EcoRI (b) assay date 7/05

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

Archives

January 2007 (24)
December 2006 (11)
November 2006 (5)

Sections

[beta-galactosidase preparation and assays \(18\)](#)
[Beta-glucuronidase \(18\)](#)
[Data \(Formatting\) \(1\)](#)
[Software discussions \(2\)](#)
[Starting materials and reagents \(1\)](#)

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)
jrh4712-82 (1)
jrh4712-84 (1)
jrh4712-85 (1)
4712-88 (1)
jrh4712-89 (1)
4712-86 (1)
jrh4712-87 (1)
4712-90a (1)


Product

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

LABTROVE AND USER DEFINED METADATA

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:



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[June 2012 \(1\)](#)
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[March 2012 \(29\)](#)

Sections
[Analytical Procedures \(8\)](#)
[Condensation Products \(5\)](#)
[Experimental Procedure \(1\)](#)
[Spectroscopic Data \(31\)](#)

Substituent
[Nitro \(8\)](#)
[Methoxy \(8\)](#)
[Bromo \(8\)](#)
[Chloro \(8\)](#)
[Methyl \(8\)](#)

Spectroscopic Method
[DSC \(5\)](#)
[ATR-FT-IR \(5\)](#)
[HPLC \(5\)](#)
[MS-ESI \(5\)](#)
[PXRD \(1\)](#)
[H-NMR \(5\)](#)
[C-NMR \(5\)](#)

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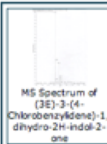
Section*
 Analytical Procedures

Metadata

key	value
Substituent	Nitro
Spectroscopic	DSC

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:



Comment on Figures

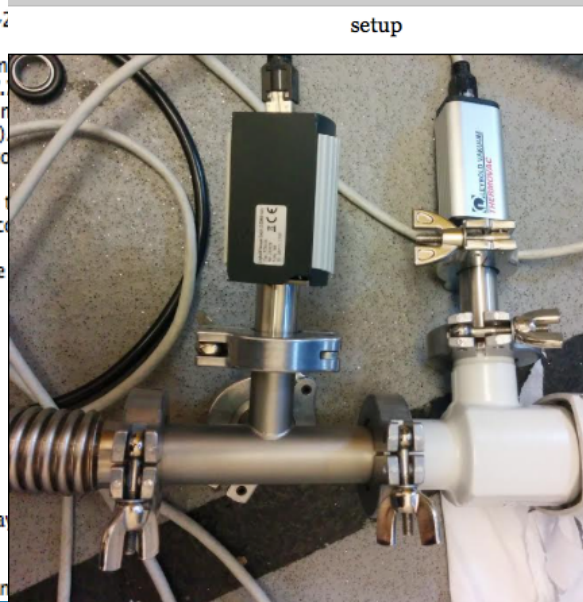
Here are main steps.

1. Oil pump - adaptor - pressure gauge. After 7 min pressure $5.0e-4$ mbar
2. Oil pump - metal tube (about 2 meters) - adaptor - pressure gauge. After 30 min pressure $5.8e-4$ mbar
3. Oil pump - trap (no alumina) - metal tube (~2 m) - adaptor - pressure gauge. After 15 min pressure $5.0e-4$ mbar
4. Oil pump - trap (no alumina) - metal tube (~2 m) - adaptor - pressure gauge. After 15 min pressure 7.
5. Oil pump - trap (no alumina) - metal tube (~2 m) - adaptor - pressure gauge. After 15 min pressure 7.
6. I have changed alumina and placed it back into the trap. After 1 h pressure $1.2e-3$ mbar
7. Then Ed moved the oil pump into the lab so we could

Here is the part which we were connecting with the better understanding.



- oil pump - trap (alumina) - metal tube (~2 m) - 4-way
- 1 closed
- pressure gauge
- gate valve - adaptor - small turbo pump - EUV chamber



Colours: [Black](#) [Blue](#) [Red](#) [Green](#) [Eraser](#) [Cancel Comment](#) [Submit Comment](#)

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08:17:37 13 Jan 17 - Frey J.G.

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setup

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Linking

Bi-directional
linking can
extended to
a group of
Trove

Jeremy Frey LabTrove ELN

Far field single atom spectra

6th September 2016 @ 07:42

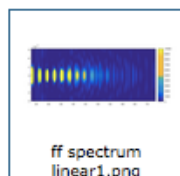
Just a footnote about what Dell has been doing in his MSc project. Ages ago we did this with the wrong transforms, and I've been meaning to do it again ever since the Artemis run where we got data from Ne which had nice detailed spectra -

Links to relevant posts are here:

A few key things from the Artemis run

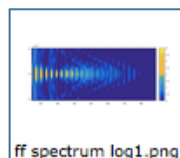
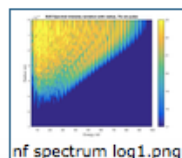
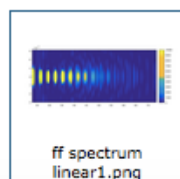
far-field quantum path interference for a single 1-D atom - Oct 2009!

We're using 7fs pulses with intensity 3×10^{14} at peak here, 800nm. Spot size is 50um. Fixed CEP, too. Predicted cutoff is 75 eV-ish.



this is the linear plot, for comparison with the Artemis stuff - you can see that we see clear harmonics up to about 45 eV, not 75.

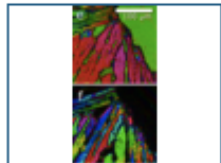
Attached Files



However, in the real SHG data, if you look at (e) and (f) it's clear that the SHG phase (f) is varying very fast compared to the line

So what's varying? A variation small given that the x and z is orientation effect, but it's very

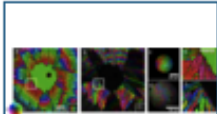
Is this obvious to anyone out like the phase jump could be causes the sign of d to change



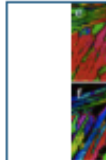
SHG_NMBA_e_and_f.jpg

[my link:NMBA properties (We

Attached Files



SHG_NMBA_all.png



SHG_NMBA_e_and_f.jpg

OneNote Online

OneDrive ▸ Documents

Research Journal 2015

HOME

INSERT

VIEW

PRINT



Tell me what you want to do

EDIT IN ONENOTE

GIVE FEEDBACK TO MICROSOFT

Find on this Page (Cmd ⌘)

+ Page

SHG CDI

NMBA properties

Jones matrices

PPLN analysis

Day 2

Phase Match's 5 Abs

Untitled Page

Paper notes while writing

NMBA properties

Thursday, 7 May 2015 10:00

Just exploring these - from Bailey93. What could the maximum delta k be?
Fig 6 has the refractive indices

$$\Delta k = k_{2\omega} - 2k_{\omega} = \frac{2\pi}{400\text{nm}} \cdot n_{2\omega} - \frac{2\pi}{800\text{nm}}$$

$$\Delta k = \frac{2\pi}{400\text{nm}} (n_{2\omega} - n_{\omega}) \quad , \quad L = 7\mu\text{m}$$

WSB Matlab Autoblog

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

[Older Entries >>](#)

Search 

fe_transmission.m

8th November 2016 @ 10:09

matlab code:

```
%Fe_transmission.m
%looking at using Iron to get differential absorption.
constants;
lambda0 = 800e-9;
q = 31:2:41;
lambda = lambda0 ./q;
stuff = 'fe';
%stuff = 'ca';
%stuff = 'k'
[eV, k, alpha] = get_index2(stuff);
l = h * c ./ (eV * e);
t = 0.5e-8; % film thickness
trans = exp(-alpha * t);
phi = k * t; %note routine returns k not delta
figure(10)
%yyaxis left
plot(1*1e9,trans)
xlabel('wavelength /nm')
ylabel('trnsmission');
yyaxis right
plot(1*1e9,phi)
ylabel('phase shift');
title(sprintf('%s film, %g nm thick, harmonics 31-41 of %g nm', stuff, t*1e9, lam
xlim([15 35])
```

This Notebook

[New Entry](#)
[Notebook Settings](#)
[Timeline View](#)
[Export Notebook](#)
[Feed \(+Comments\)](#)

Archives

November 2016 (6)
August 2016 (3)
May 2016 (2)
April 2016 (1)
March 2016 (5)
January 2016 (8)
November 2015 (5)
October 2015 (5) [\(more\)](#)

Authors

Brocklesby W.S. (340)

Sections

[jets and cells](#) (1)
[Matlab Autoblogging](#) (339)

Tools

[Show/Hide Keys](#)

Jeremy Frey Lab

20

13/01/2017

Text Analysis and Lookup Services

Anti-Microbial Resistance Network

Notebook for AMR projects

Entry published

Previous Entry >>

Search

Example of Chemistry

13th January 2017 @ 09:07

Ethanol and Water mixtures with the addition of a small amount of toluene

Jeremy Frey | Edit Entry | Test | Comments (0)

Chemspider Info

Ethanol Water toluene Delete

toluene (Confidence: 0.94697, Timestamp: 2017-01-13 09:09:28)

id: 1108

molecular weight: 92.1384

molecular formula: C_7H_8

smiles: Cc1ccccc1

inchi: InChI=1/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3

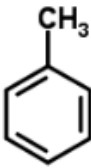
inchikey: YXFVVABEGXRONW-UHFFFAOYAT

average mass: 92.1384

monoisotopic mass: 92.062599

nominal mass: 92

common name: Toluene



This Entry

Permalink
URI
URI Label
Revision:
Add to L
Edit Entry
Export:
XML

This Notebook

New Entry
Notebook
Timeline
Export Notebook
Feed

Archive

January 2017
October 2016
December 2016

Author

Jeremy Frey

Section

Conference
Test (2)

Tools

Show/Hide

Current user: Andrew Milsted | Log Out All Blogs | Help

BlogMyData

HiGEM Blog

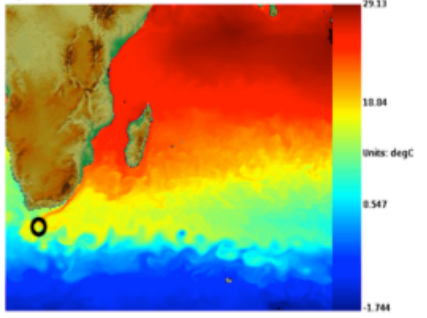
Blog for the HiGEM community

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: 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

Godwaz test site for BlogMyData > HiGEM XBYLR Monthly means > OCtrl/ Temperature.
 Time: 2010-08-16T00:00:00.000Z
 Depth: 3.050000190734863 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
 Permalink
 URI
 URI Label
 Revisions
 Export:
 XML (With Files)
 PNG Image

This Blog
 New Post
 Blog Settings
 Timeline View
 Exhibit View

Archives
 October 2010 (3)
 September 2010 (2)
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Sections
 ahm2007 (13)

Viztype
 StaticMap (5)
 StaticMapWithPoint (2)
 Animation (6)

Dataset
 HiGEM_XBYLR_MONTHLYMEAN (13)

Variablestandardname
 OCtrl/ Temperature. (6)
 OCtrl/ Salinity. (2)
 Density (5)

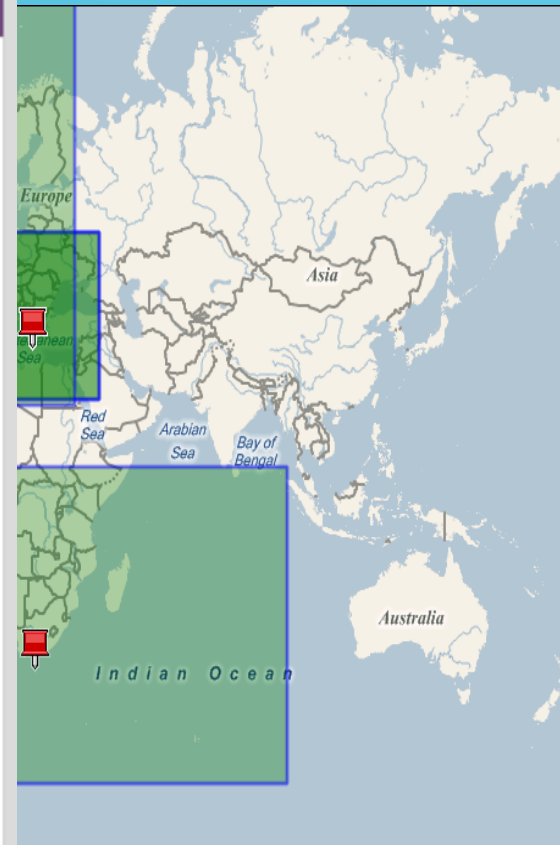
Calendarsystem
 360 Day (13)

Elevationunits
 M (13)

Elevationpositive
 Down (13)

Tools
 Show/Hide QR Code
 Show/Hide Keys

BlogMyData Project - Godiva



Tpp Methyl ester Hydrolysis:- Methord 2

9th April 2009 @ 16:50

Lab Note Book Or Experiment Code: FDH-5405-E7P26

Post Type: Methord_2

Procedural Step: Methord_2

Date Of Experiment: 27-11-08

Experiment Name: Tpp_Methyl_ester_Hydrolysis

Experiment Code:FDH/5405/E7P26

Date of Experiment:27/11/08

- reaction mixture added to 100ml of DCM
- solid formed...dissolved in DCM/MeOH + water and evaporated to near dryness
- re dissolved in 200ml chloroform+20ml MeOH, sonicated most dissolved.
- 30ml water added myselfs leading to solid problems and poor separation seen.
- 100ml water added now gives clear layer with myselfs below
- transferred to bigger 500ml sep funnel.



this picture taken directly after transference

- approx. 30ml 2M hydrochloric added to give emitate separation. and turn porphyrin protonated green.
- much better behaved now....lovely shade of green too.



protonated porphyrin with 2M HCL

- HCL reextracted with 100ml CHCl₃.
- fluffly brown noted between interface. contaminant?
- organic rinsed 5 times 100ml water. first rinse turns it back to purple



now purple organic with aqueous

- water re-extracted into chloroform 100ml and rinse 5 times H₂O.
- organic fractions combined and dried over anhydrous sodium sulfate



Jeremy Frey Lab@rove ELN

27-11-08 (2)

30-11-08-1-12-08 (1)

Experiment Name

[Preparation Of Fulleropyrrolidin](#)
[Alcohol:-Planning And Safety \(8\)](#)
[Preparation Of N-Glycine](#)
[\(amino-Ethoxy-Ethanol\) Tert](#)
[Butyl Acetate \(4\)](#)
[Preparation Of P-tert Butyl](#)
[\(bis\(cyanomethoxy\)dihydroxy\)](#)
[Calix \(2\)](#)
[Preparation Of Mono Para Methyl](#)
[Ester Meta Tetra Phenyl](#)
[Porphyrin \(10\)](#)
[Removal Of A Protecting Group](#)
[To Give \[\(hydroxyethoxy\)ethyl](#)
[Amino\] Acetic Acid Repeat Ed](#)
[\(2\) \(4\)](#)
[Removal Of A Protecting Group](#)
[To Give \[\(hydroxyethoxy\)ethyl](#)
[Amino\] Acetic Acid \(5\)](#)
[Preparation Of Fulleropyrrolidin](#)
[Alcohol \(repeat 2\) \(3\)](#)
[Preparation Of Fulleropyrrolidin](#)
[Alcohol \(repeat 2\) \(1\)](#)
[Tpp Methyl Ester Hydrolysis \(5\)](#)

Chemical

[Dichloromethane \(1\)](#)
[Triethylamine \(1\)](#)
[2-\(2-Aminoethoxy\)ethanol \(1\)](#)
[Template \(1\)](#)
[TertButylbromoacetate \(1\)](#)
[Tert Butyl 2 \(2 \(2](#)
[Hydroxyethoxy\)ethylamino\)acetate](#)
[\(1\)](#)
[SodiumHydroxide1M \(1\)](#)
[Buckminsterfullerene \(1\)](#)
[Paraformaldehyde \(1\)](#)
[Toluene \(1\)](#)
[2-\(2-\(2-](#)
[hydroxyethoxy\)ethylamino\)acetic](#)
[Acid \(1\)](#)
[Fulleropyrrolidin Alcohol \(1\)](#)
[Pyrrole \(1\)](#)
[Methyl4-formylbenzoate \(1\)](#)
[Benzaldehyde \(1\)](#)
[Chloroform \(1\)](#)
[BoronTrifluorideEtherate \(1\)](#)
[2,3-Dichloro-5,6 Dicyano-](#)
[1,4-Benzquinone \(1\)](#)
[5-4-Methyl Benzoate](#)
[10,15,20-tri Phenyl Porphyrin](#)
[\(4\)](#)

Accessibility
and Usability

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13/01/2017

Templates

Jeremy Frey LabTrove ELN

RESEARCH ARTICLE

Open Access



Effects of using structured templates for recalling chemistry experiments

Cerys Willoughby*, Thomas A. Logothetis and Jeremy G. Frey

Abstract

Background: The way that we recall information is dependent upon both the knowledge in our memories and the conditions under which we recall the information. Electronic Laboratory Notebooks can provide a structured interface for the capture of experiment records through the use of forms and templates. These templates can be useful by providing cues to help researchers to remember to record particular aspects of their experiment, but they may also constrain the information that is recorded by encouraging them to record only what is asked for. It is therefore unknown whether using structured templates for capturing experiment records will have positive or negative effects on the quality and usefulness of the records for assessment and future use. In this paper we report on the results of a set of studies investigating the effects of different template designs on the recording of experiments by undergraduate students and academic researchers.

Results: The results indicate that using structured templates to write up experiments does make a significant difference to the information that is recalled and recorded. These differences have both positive and negative effects, with templates prompting the capture of specific information that is otherwise forgotten, but also apparently losing some of the personal elements of the experiment experience such as observations and explanations. Other unexpected effects were seen with templates that can change the information that is captured, but also interfere with the way an experiment is conducted.

Conclusions: Our results showed that using structured templates can improve the completeness of the experiment context information captured but can also cause a loss of personal elements of the experiment experience when compared with allowing the researcher to structure their own record. The results suggest that interfaces for recording information about chemistry experiments, whether paper-based questionnaires or templates in Electronic Laboratory Notebooks, can be an effective way to improve the quality of experiment write-ups, but that care needs to be taken to ensure that the correct cues are provided.

Keywords: Templates, Experiments, Experiment record, Context, ELN, User experience, Study

Dashboard

Search All

Your Notebooks

- UltraFast Xray Group
- Ultrafast TeraHertz
- MatLab Output

Your Subscriptions

- UltraFast Xray Group

Your Draft Entries

- General solution for quantitative dark-field contrast imaging with grating interferometers Last Edited: 2nd December 2014 @ 17:10 in UltraFast Xray Group (edit entry)
- Lensless diffractive imaging with ultra-broadband table-top sources: from infrared to extreme-ultraviolet wavelengths Last Edited: 11th October 2014 @ 18:52 in UltraFast Xray Group (edit entry)
- Image Data Base Last Edited: 27th January 2014 @ 21:09 in UltraFast Xray Group (edit entry)

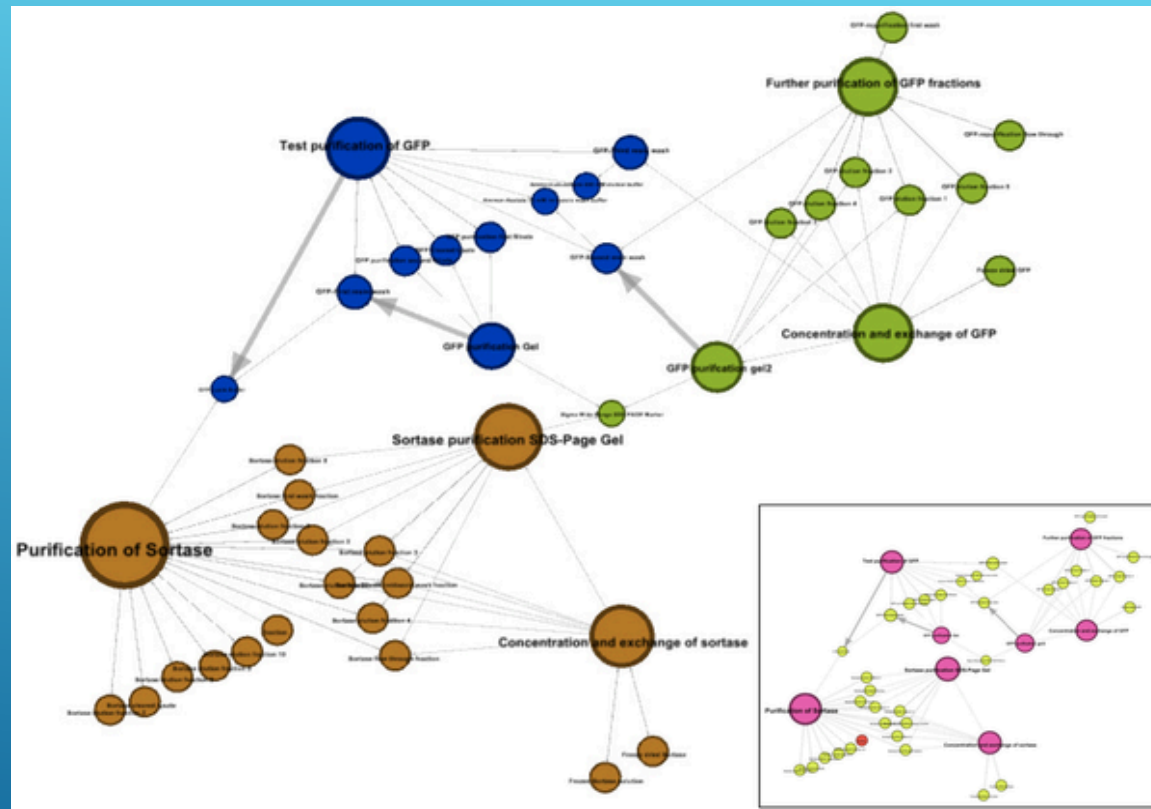
Your Recent Entries

- Pumps update 11th January 2017 @ 23:42 in UltraFast Xray Group
- Pump Exhaust 11th January 2017 @ 16:15 in UltraFast Xray Group
- Lab Water Supply 11th January 2017 @ 15:40 in UltraFast Xray Group
- First XUV of the year 11th January 2017 @ 15:34 in UltraFast Xray Group
- Hyun-Su PhD 5th January 2017 @ 10:31 in UltraFast Xray Group
- Laser Switch On Jan 3rd 2017 5th January 2017 @ 09:58 in UltraFast Xray Group
- More pumping problems... 5th January 2017 @ 09:50 in UltraFast Xray Group
- Pumps again 5th January 2017 @ 02:49 in UltraFast Xray Group
- I14 commissioning call: Deadline 27th January 2017 19th December 2016 @ 14:06 in UltraFast Xray Group
- VUV-CE3 photoelectron spectroscopy update 14th December 2016 @ 14:55 in UltraFast Xray Group



discussion

Figure 7. Visualization of posts as a network of resources.



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>

Jeremy Frey LabTrove, LLN

ARCHIVE

Jeremy Frey LabTrove ELN

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13/01/2017

LabTrove Open Notebooks Mat Todd's Malaria Project

Praziquantel – Open Science

Products of an Imperial Drug-Resistant Collaboration

Praziquantel Project

- Introduction
- Project updates
- Project discussion
- ATC links

Student Collaboration

- Hydrolysis of PZQ
- Resolution of PZQ
- Synthesis of Racemizing 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

19th August 2012 @ 10:08

Synthesis of SC2-1 from tryptamine and 4-nitrobenzaldehyde

IRAC

Procedure followed

Racemization of PZQ and PZQamine

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

13th April 2011 @ 14:07

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

Racemic Resolution of Praziquantel and Praziquanamine

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

2nd August 2012 @ 09:08

Hazard and Risk Assessment:

Procedure

To a cooled solution of MNR7-6 (7.1 g, 35.13 mmol) in DCM (370 mL) at 0°C was added triethylamine (2.24 mL, 16.26 mmol) and benzoyl chloride (8.48 mL, 38.62 mmol). The solution was stirred for 14 hours at room temperature.

In the evening, the reaction was quenched with water (40 mL) and stirred for 30 minutes then the

Hydrolysis of PZQ

Hydrolysis of PZQ – WGPZQ101

21st June 2012 @ 10:12

Preliminary step in producing enantiopure PZQ: acid hydrolysis of

See also:

- Hydrolysis of PZQ – Standard Conditions (K9-PZQ-1001)
- Hydrolysis of rac-PZQ (K9PQ-130)
- Hydrolysis of rac-PZQ (K9PQ-140)
- Optimizing the acid cleavage conditions

Procedure:

rac-PZQ (4.0 g, 12.8 mmol, 90%:10%) was dissolved in a mix

KAB17-1 (N-benzoyl PZQ analogue). Peptide Acetal KAB6-1: 373.1 mg (0.936 mmol), toluene: 37 mL, TFOH: 4.14 µL (0.047 mmol, 5 mol%).

KAB13-2 (PZQ). Peptide Acetal KAB5-2: 394.2 mg (0.974 mmol), toluene: 39 mL, TFOH: 4.32 µL (0.049 mmol, 5 mol%).

Monitoring the Reaction Progress by TLC

The progress was monitored by TLC of the reaction mixture against the relevant starting material, the expected product and the completely cyclised product. All TLCs were eluted with EtOAc/hexane, 5:3, v/v and stained with KMnO_4 .

LabTrove Notebooks

The screenshot shows a grid of six notebook thumbnails from the LabTrove interface. The thumbnails are arranged in two rows of three. The top row includes 'Pictet-Spengler route to Praziquantel' and 'Racemization of PZQ and PZQamine'. The bottom row includes 'Racemic Resolution of Praziquantel and Praziquanamine' and 'Hydrolysis of PZQ'. The 'Introduction' thumbnail is also visible. Each thumbnail features chemical structures and text describing the experiment.

Select
entries
(all)

Zip and send to
repository

Export as HTML
“static” copy

DataCite DOI

The collage consists of six screenshots from the DataCite website:

- Top Left:** DataCite homepage with the tagline "Helping you to find, access, and reuse data". It features a job opportunity for a Technical Officer and a sidebar with links like "Why data", "What Data", and "What we d".
- Top Middle:** Another view of the DataCite homepage, similar to the first one.
- Top Right:** "Metadata Search beta" interface. It shows a search bar and a list of search results for the compound (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one.
- Bottom Left:** "DataCite Content Service Beta" page for the DOI 10.5258/POC/LT/R/1. It provides citation information and alternate identifiers.
- Bottom Middle:** "Reports" page for the same compound, showing a table with columns for Condensation, Product, and Oxindole, and a section for ATIR-FT-IR Spectrum.
- Bottom Right:** "LabTrove" interface, showing a search bar and a list of notebooks related to the compound.

Below the screenshots, the following text is displayed:

DataCite | Helping you to find, access,...

DataCite | Helping you to find, access,...

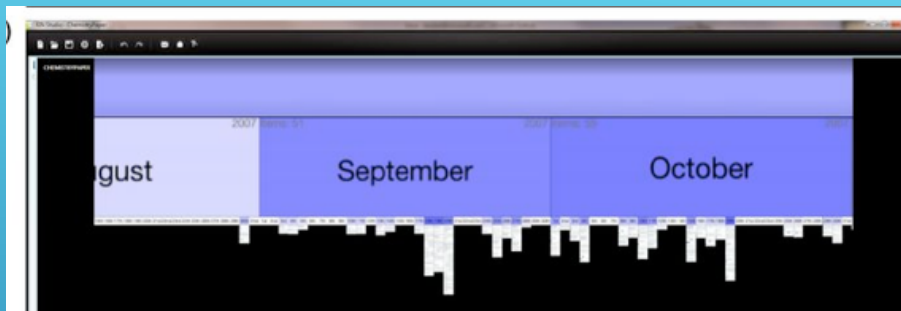
<http://search.datacite.org/ui/?q=Tiz...>

10.5258/POC/LT/R/1

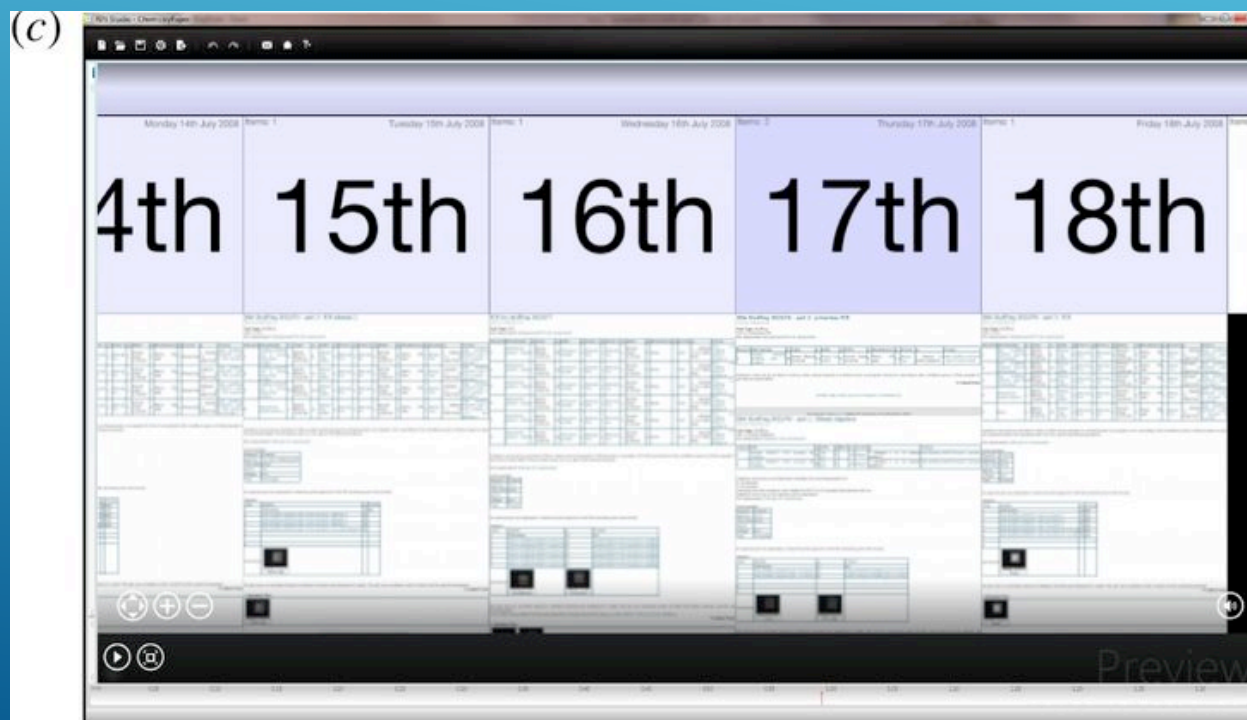
Reports

LabTrove

http://royalsocietypublishing.org/content/371/1983/20120090.jnl_roysco_tab_art



Use of Deep Zoom technique



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

Impact on researchers

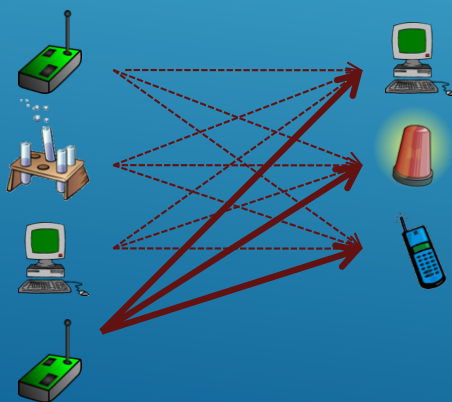
- ▶ ELN is not something to be considered in isolation
- ▶ Needs to be considered as part of a whole (digital) lab ecosystem

LAB ECOSYSTEM

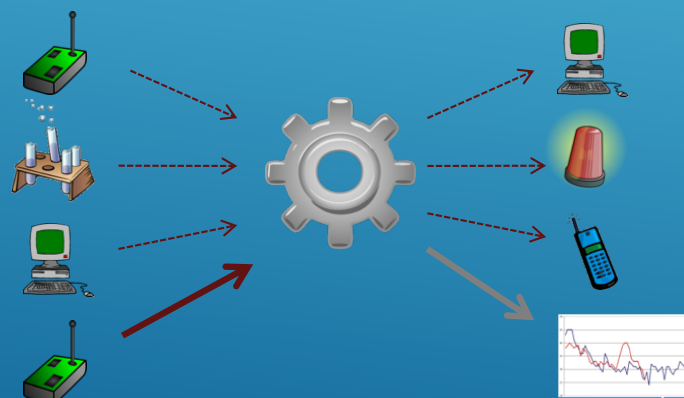
Middleware: The SRF LabBroker Software:

Get the data into the Trove before the users even look

- Without middleware



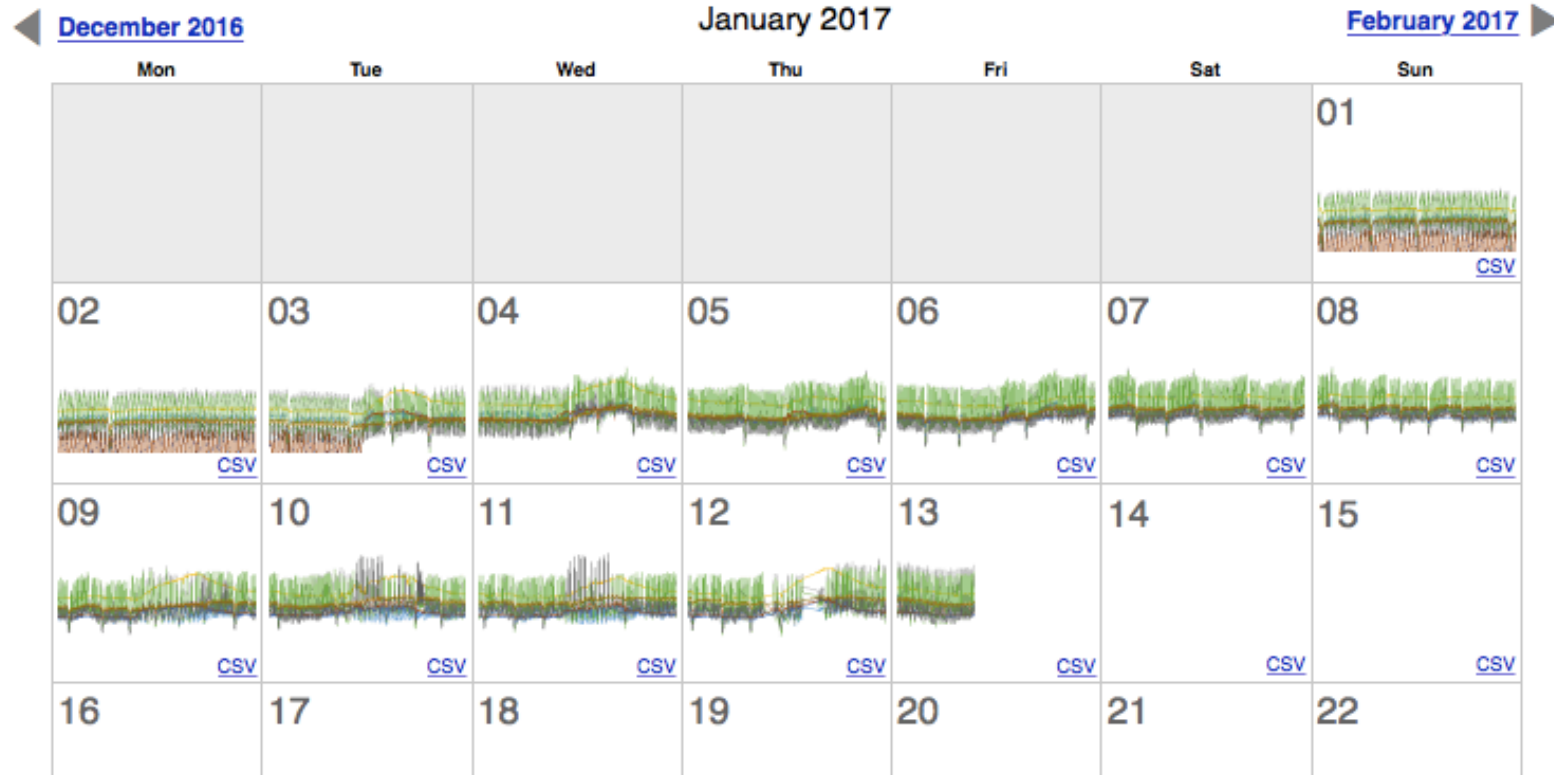
- With middleware



DataBroker

[Home](#) > [Devices](#) > [Temperature sensors \(Bench\) in 46:1047](#) > January 2017

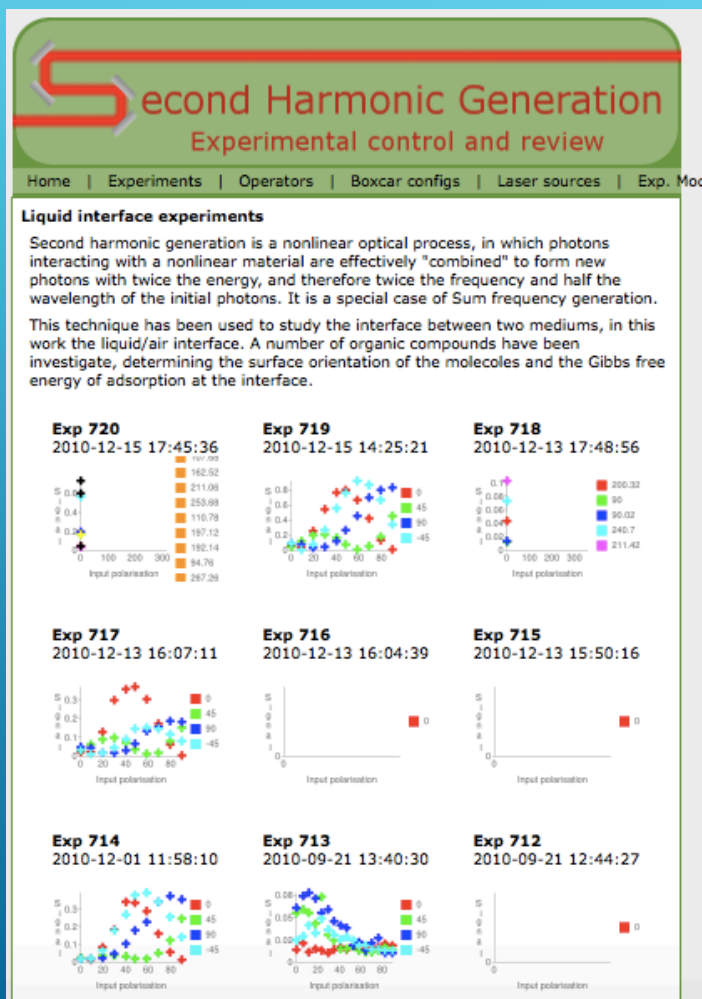
Temperature sensors (Bench) in 46:1047



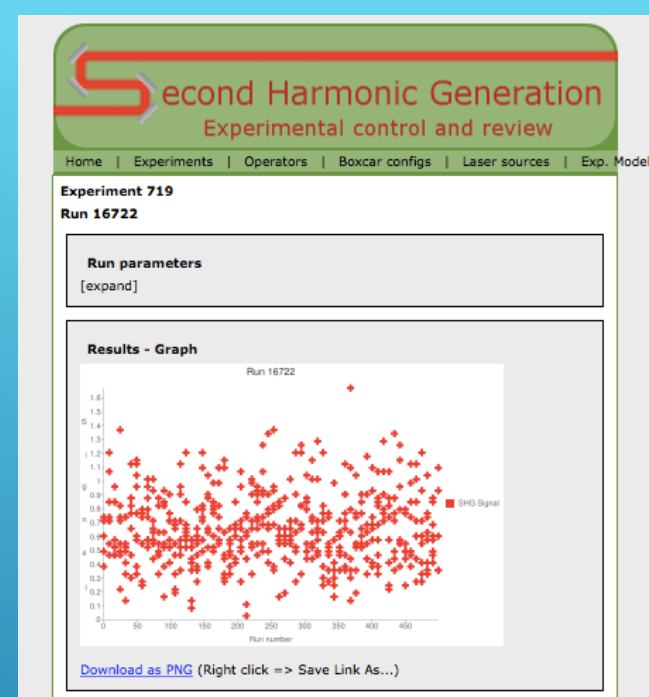
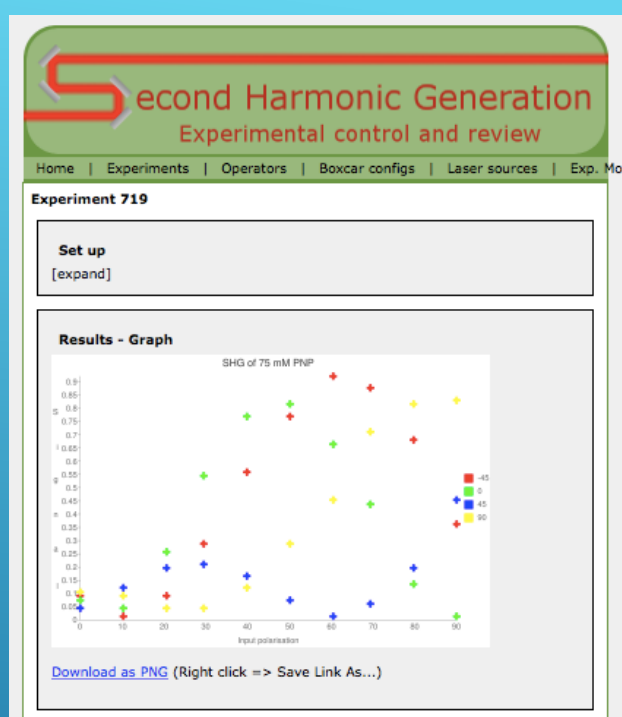
SLACK

The screenshot shows a Slack interface for a workspace named 'xraygroup'. On the left sidebar, there is a list of channels: #proposals, #random, #theitalianjob, #trliterature, and #xrayblog. Below these are direct messages with slackbot, jgf (you), adam, bill, bill, russell, bill, russell, phorak70, dell, and ed (highlighted). At the bottom of the sidebar is an 'Invite people' button.

The main window shows a channel view for '@ed'. The header indicates '@ed' is active, with a profile picture and name 'Ed Jager'. Below the header is a line graph titled 'Today' showing data for various sensors. The graph has a legend with items like 'Infrared Left', 'Aspen's Box', 'B.L.P.', 'Thermist', 'Cooler Left', 'Aspen's Box', 'B.L.P.', 'Cooler Right', 'Tetra Station', and 'Tetra Top'. The graph shows multiple data series with a red line representing a trend. Below the graph is a 'Downloads' section with links to 'Raw data file (2017-01-09)' and 'Processed data file (2017-01-09)'. Below the graph is a message from 'ed' at 9:36 AM, stating 'uploaded this image: Laser_On.png'. Below the message is another line graph titled 'DataBroker' showing 'Temperature sensors (Bench) in 46:1047'. This graph has a legend with items like 'Infrared's Box', 'B.L.P.', 'B.L.P.', 'Thermist', 'Cooler Left', 'Aspen's Box', 'B.L.P.', 'Cooler Right', 'Tetra Station', and 'Tetra Top'. The graph shows multiple data series with a red line representing a trend. Below the graph is a 'Message @ed' input field.



Jeremy Frey LabTrove ELN



Experimental data & analysis available via a database

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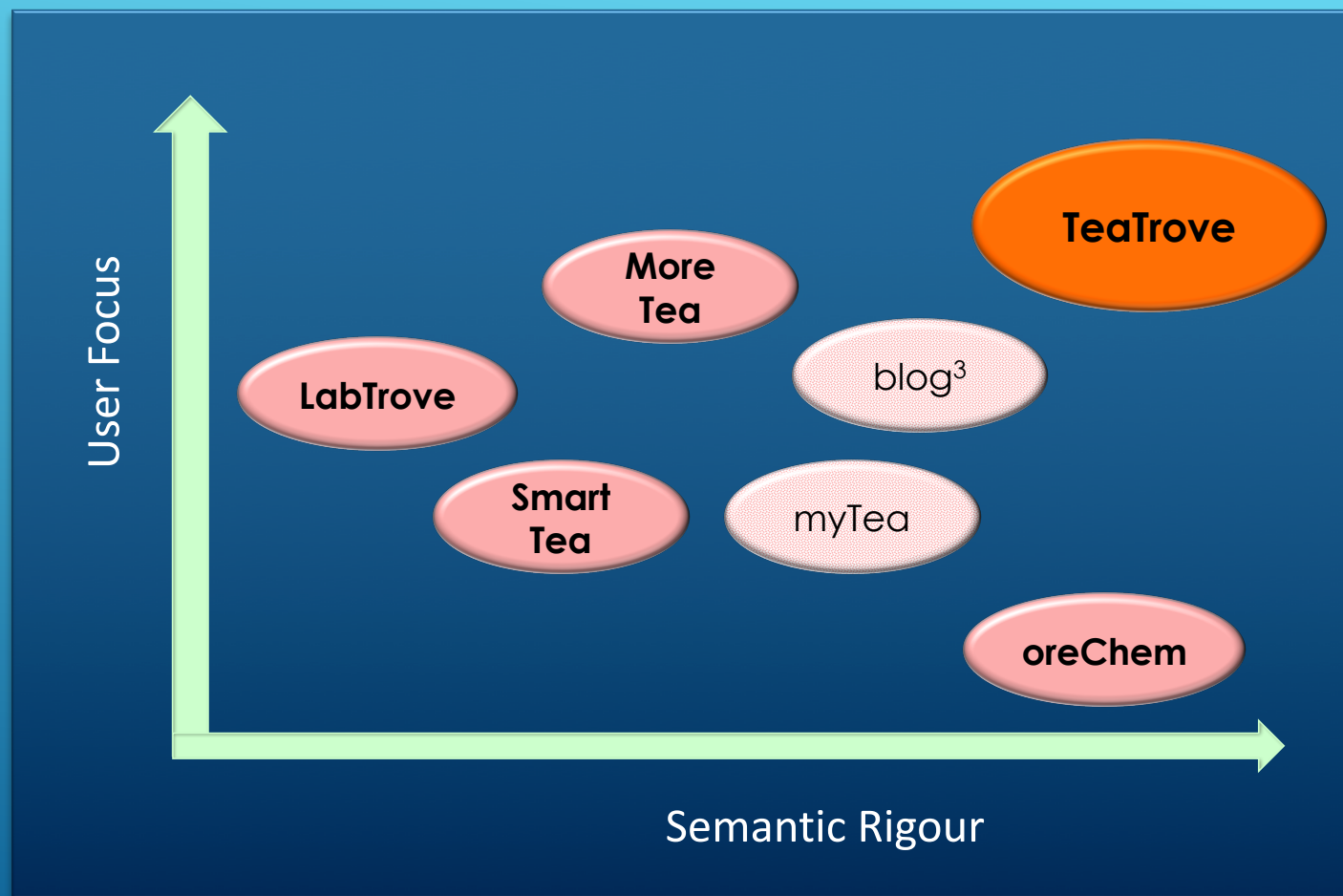
13/01/2017

FUTURE

Jeremy Frey LabTrove ELN

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PLATFORMS

Jeremy Frey Lab@rovet ELN

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Ontology

Research to Product



cc: quinn.anyia - <https://www.flickr.com/photos/53326337@N00>

We must speed up the knowledge discovery process



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

Thank you for listening



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From *The New Yorker Book of Technology Cartoons*.

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