

Science Ajar

"The opportunity of Open Science"



Great Expectations

*Supporting Inter-, Multi- and Open-
Collaborations*

Jeremy Frey

Chemistry

Faculty of Natural and Environmental Science

University of Southampton

&

Champion of the Digital Economy IT as a Utility Network

Talk Outline

- Discuss my experience in some of the research projects I have been involved with over the last 10 years
- Move to increasing openness especially with research data to facilitate collaborations
- How e-Science and related technology can help
- Social vs Technical – Rewards!

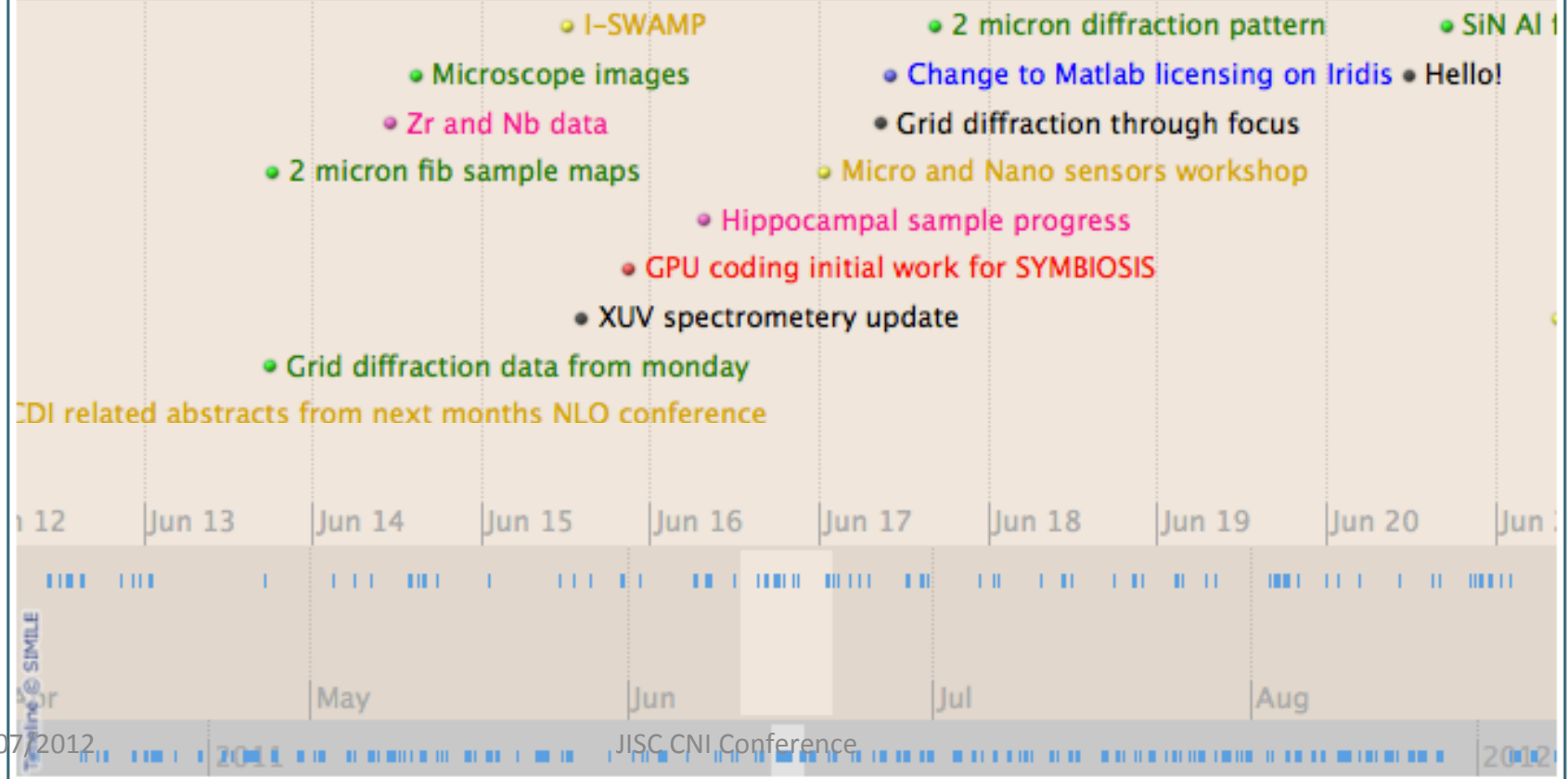
UltraFast Xray Group

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Timeline



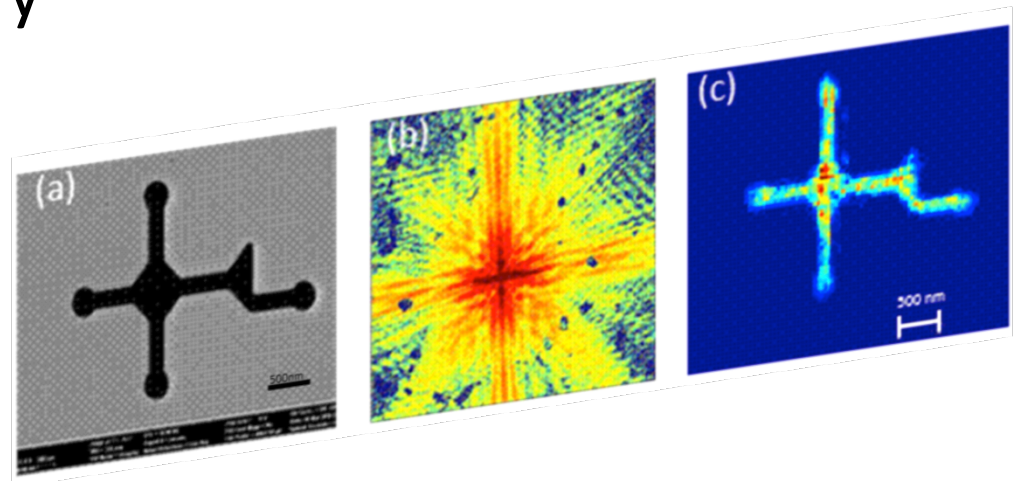
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JISC CNI Conference

2012

Inter or Multi-disciplinary Research *(Is there a difference?)*

- CombeChem
 - Chemistry, Computer Science, Statistics
- Laser based ultrafast Soft X-Ray Imaging
 - Physics and Chemistry
- IT as a Utility
 - Digital Economy
 - Social & Technical Disciplines



CabinetOffice

Open Data White Paper and Departmental Open Data Strategies

28 June 2012

COVERITL
Powering the world's real-time

Open Data White Paper
Replay

Research Information

THE ROYAL SOCIETY

Expanding access to research
Report of the Working Group on Expanding Access to Research – the Finch Group

The report of the Working Group chaired by Dame Janet Finch recommends a programme of action to enable more people to benefit from research. Better, faster communication of research results arising from research. Better, faster communication of research results arising from research. Better, faster communication of research results arising from research.

The internet has brought much better access to research. But the full benefits of the digital and online world are not being realised, especially for business, the professions, and the general public. The key to realising the potential of the digital world is a worldwide open access regime. The key to realising the potential of the digital world is a worldwide open access regime.

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

- Scientists need to be encouraged to share their data 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
- EPUB and Kindle version**
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

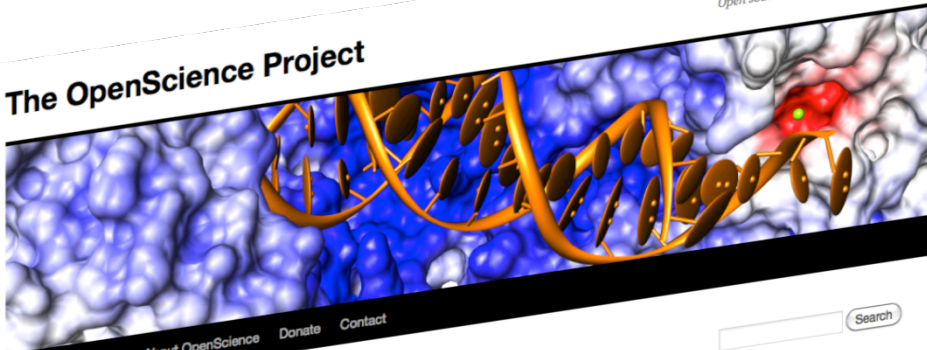
Intelligent Open Access to Data

06/07/2012

JISG CNI Conference

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The OpenScience Project



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Computational Chemistry Highlights

Posted on March 7, 2012 by Dan Gezeiter

Computational Chemistry Highlights (CCH) is an interesting new [overlay journal](#) that identifies important contributions to the field of computational and theoretical chemistry published within the last 1-2 years. I'm involved in the journal, concentrating on recent developments and papers in computational chemistry and theoretical mechanics. The journal will eventually get to a point where we can help us all keep up on advances in the field that

Blogroll

- arXiv.org e-Print archive
- badscience
- blum (Damaris Gish)

**Access to the discussion
and the means to
reproduce the analysis**

Computational Chemistry Highlights

Important recent papers in computational and theoretical chemistry
A free resource for scientists run by scientists

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SATURDAY, JUNE 23, 2012

Accurate Predictions of Nonpolar Solvation Free Energies Require Explicit Consideration of Binding-Site Hydration

Samuel Genheden, Paulius Mikulskis, LiHong Hu, Jacob Kongsted, Pär Söderhjelm, and Ulf Ryde *Journal of the American Chemical Society* 2011, 133, 13092 (Paywall)

ab initio prediction of protein-ligand binding free energies
Fast computers and clever algorithms have made it possible to calculate protein-ligand binding free energies. PCM (Polarizable Continuum Model) theory that have been shown to give accurate gas phase binding energies. However, the combined use of *ab initio* and PCM (without the solvation methods of choice for most *ab initio* studies have now also been implemented for protein size systems. However, the combined use of *ab initio* and PCM (without

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NATURE | PERSPECTIVES

The case for open computer programs

Darrel C. Ince, Leslie Hatton & John Graham-Cumming

Affiliations | Contributions | Corresponding author

Nature 482, 485–488 (23 February 2012) | doi:10.1038/nature10836

Received 09 May 2011 | Accepted 05 January 2012 | Published online 22 February 2012

Scientific communication relies on evidence that cannot be entirely included in publications, but the rise of computational science has added a new layer of inaccessibility. Although it is now accepted that data should be made available on request, the current regulations regarding the availability of software are inconsistent. We argue...

Subject terms: Computing science • Information technology

日本語要約

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Crossref (0) Scopus (5) Web of Science (2)

Selected feature

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How three-dimensional printers are opening new worlds to researchers.

See complete feature

BBC News – Higgs boson-like particle discovered

Including the code?

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Research Universities and the Future of America

National Academies Press

America is driven by innovation — advances in ideas, products, and processes that create new industries and jobs, contribute to our nation's health and security, and support a high standard of living. In the past half-century, innovation itself has been increasingly driven by educated people and the knowledge they produce. Our nation's primary source of that knowledge is research universities. Our research continues to be our research.

However, these institutions have outdated streams and antiquated policies. It is essential to maintain the unique partnership that has existed between government, the states, and industry. In doing so, we will create jobs, increased incomes, and

This PDF is available from The National Academies Press at http://www.nap.edu/catalog.php?record_id=13433

An Interim Report on Assuring DoD a Strong Science, Technology, Engineering, and Mathematics (STEM) Workforce



ISBN
978-0-309-26004-6

22 pages
8.5 x 11
2012

Committee on Science, Technology, Engineering, and Mathematics Workforce Needs for the U.S. Department of Defense and the U.S. Defense Industrial Base; Board on Higher Education and Workforce; Division on Policy and Global Affairs; Division on Engineering and Physical Sciences; National Academy of Engineering; National Research Council

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BBC News - 'Show Your Working': What 'ClimateGate' means

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'Show Your Working': What 'ClimateGate' means

VIEWPOINT
Mike Hulme

The "ClimateGate" affair has seen documents hacked or leaked from a climate research institute's web. But what does it mean for the work of Mike Hulme and Jerome Ravetz, who have made a concerted effort to expand our understanding of the process of climate change?

As the repercussions of ClimateGate reverberate through the virtual community of citizens, we believe it is both important and urgent to reflect on what this moment is telling us about the practice of science in the 21st Century.

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Methods are as important as the data

Byte Size Biology

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

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Home > Science, Structural biology > Structuregate?

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 not necessarily finished. Very little detail was given, but the structures are tied to a paper reported by the Birmingham group.

The structures' PDB IDs are 1CMW, 1DF9/2QID, and 2QID. They are still in the database.

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CRU Scientific Assessment Panel announced

Mon, 22 Mar 2010

Lord Oxburgh FRS, a member of the CRU Scientific Assessment Panel to examine the impact of climate change on the UK, has been appointed to the panel.

His appointment has been announced by the CRU. The panel will have access to all the data and information available to the CRU and will be responsible for assessing the impact of climate change on the UK.

Announcing the appointment of Lord Oxburgh to the panel is a significant step forward for the CRU. The panel will be responsible for assessing the impact of climate change on the UK and will be responsible for providing advice to the CRU on how to best manage the risk of climate change.

We are delighted that a renowned scientist of the standing of Lord Oxburgh has agreed to chair this very strong independent panel and await its findings with interest. Colleagues in CRU have committed themselves to providing any support required by the panel.

The panel members are: Prof Huw Davies, Professor of Physics at the Institute for Atmospheric & Climate Science at ETH Zürich; Prof Kerry Emanuel,

Pay for privacy? Should Publicly funded research always be free?

If published obligation to make all workings available.

The academics media profile!

06/07/2012

JISC CNI Conference

JOC *Editorial*
pubs.acs.org/joc

Reporting Analytical Data

The integrity of science as a discipline rests on the ability of scientists to reproduce the claims of others. For organic chemistry, this requires that experiments be described in sufficient detail so a well-trained colleague can repeat published procedures with similar results. While none of the organic chemistry journals go to the same lengths as *Organic Syntheses*, where each procedure must be reproduced as described in an independent laboratory before publication, most ask that authors provide sufficient detail so that the procedures can be reproduced and provide sufficient data to establish the structures of new compounds that are reported. This information is necessary for the review process and for readers who want to base their experiments on published work.

The Journal of Organic Chemistry has been establishing guidelines for authors to ensure that the data provided in manuscripts are sufficient to establish the structures of new compounds. In examining manuscripts, if the data cannot be done, the manuscripts were deactivated because the authors did not provide sufficient reports for high-resolution mass spectra or combustion analyses. By June of 2009, 13 of these manuscripts had been published in other journals. In six cases, the original data were replaced by a new set that was consistent with the structures. In the other seven publications, the inconsistent data were left unchanged, were removed, or were replaced with another set of inconsistent data or data obtained by another analytical technique was substituted. Four of the manuscripts were submitted to other journals within only a few days after being deactivated by JOC.

While the number of manuscripts that JOC deactivated in 2008 because of unsatisfactory data and were subsequently published elsewhere was small, it is deeply disturbing that about a third of those authors chose to ignore the problems pointed out by JOC and submitted their manuscripts to other journals without adequately resolving the issues surrounding the data they originally reported. All of these manuscripts were submitted from academic institutions. The responsibility for this behavior clearly rests on the senior authors, who are setting a horrible example for their young colleagues.

C. Dale Poulter
Editor-in-Chief

The integrity of science as a discipline rests on the ability of scientists to reproduce the claims of others.

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sufficient detail so that the procedures can be reproduced and provide sufficient data to establish the structures

This information is necessary for the review process to base their experiments on published work.

Methods are as important as the data

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The Open Science Grid

The Open Science Grid (OSG) advances science through open distributed computing. The OSG is a multi-disciplinary partnership to federate local, regional, community and national cyberinfrastructures to meet the needs of research and academic communities at all scales.

Technical information:

- [Accounting](#)
- [Assessment](#)
- [Blueprint](#)
- [CampusGrids](#)
- [Council](#)
- [Documentation](#)
- [DocumentationTeam](#)
- [Education](#)
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Contacts: The Open Science Grid can be contacted through the Executive Director: [Lothar Bauerdick](#), Project PI: [Miron Livny](#) or Council Chair: [Ruth Pordes](#)

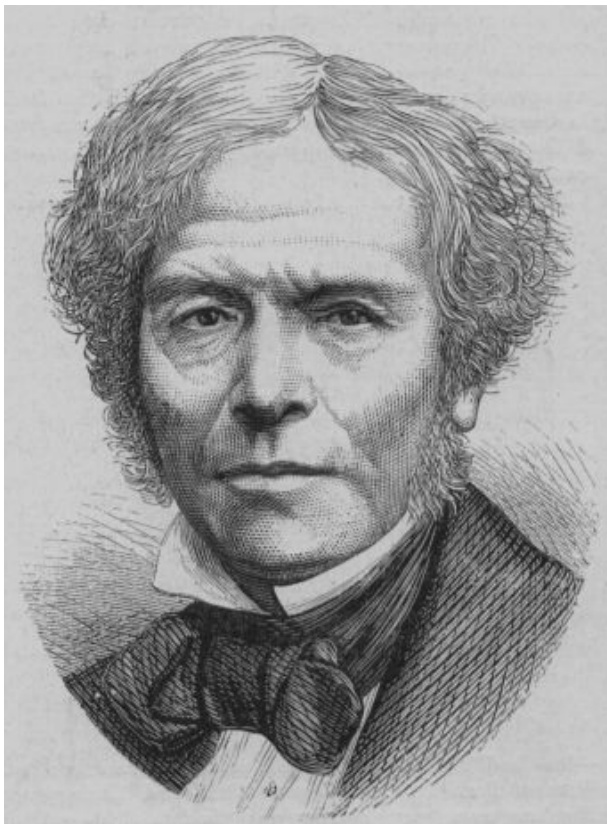
Is this really Open?

OPEN SCIENCE & OPEN DATA

ON BEING A SCIENTIST

A GUIDE TO RESPONSIBLE CONDUCT IN RESEARCH

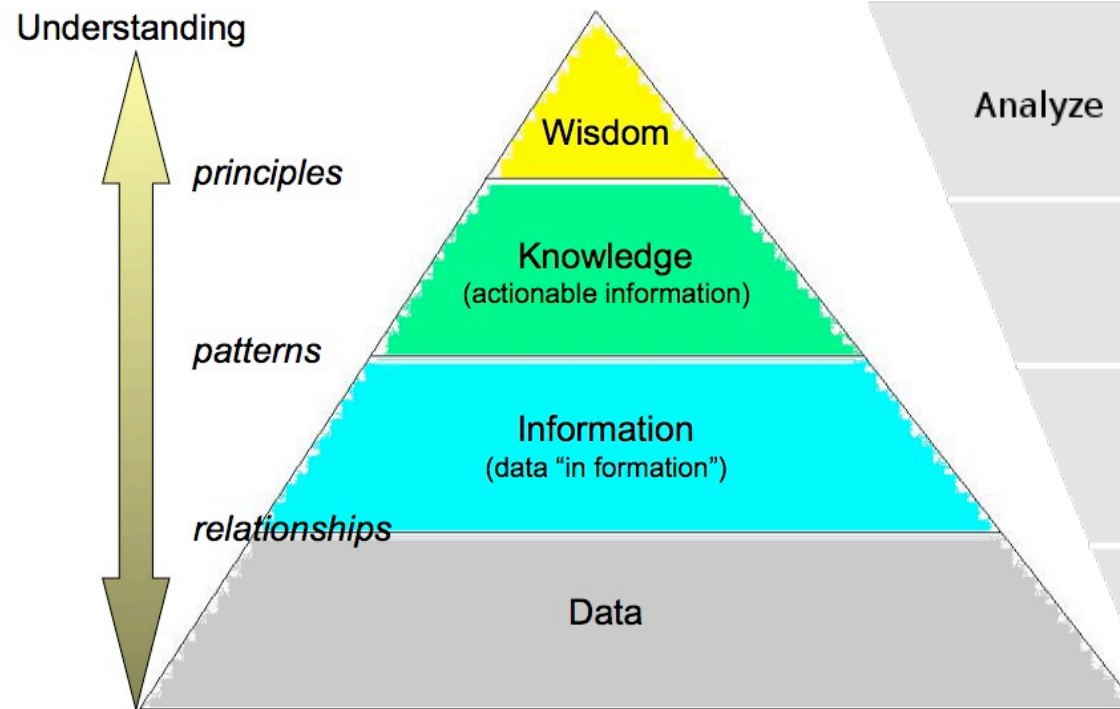
T H I R D E D I T I O N



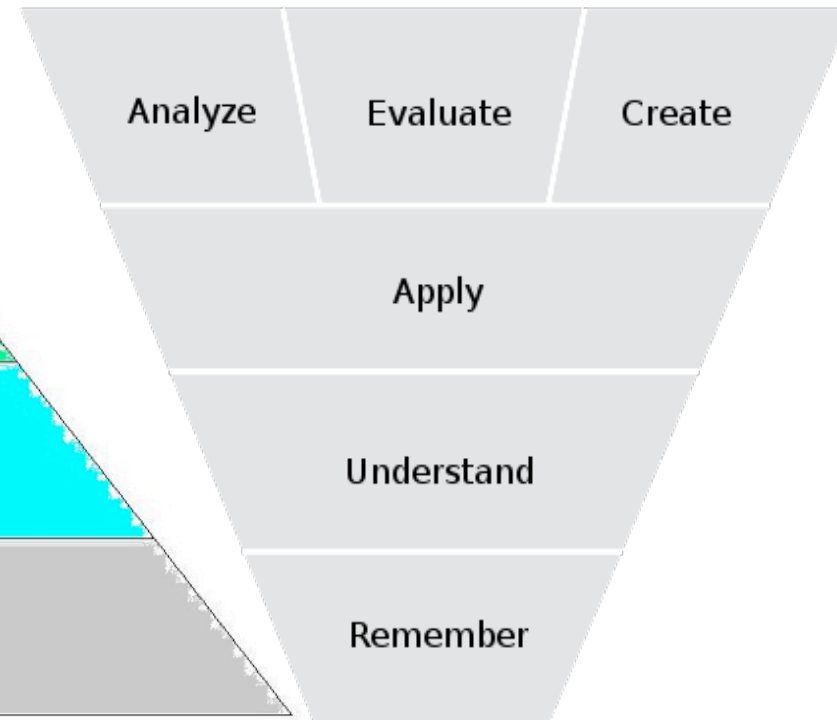
Faraday's laboratory notebooks are also remarkable in the amount of detail that they give about the design and setting up of experiments, interspersed with comments about their outcome and thoughts of a more philosophical kind. All are couched in plain language, with many vivid phrases of delightful spontaneity....

Peter Day, 'The Philosopher's Tree: A Selection of Michael Faraday's Writings'

DIKW



Bloom's Taxonomy



Adapted from: Awad & Ghaziri and Bellinger, Castro, & Mills

http://en.wikipedia.org/wiki/Bloom's_Taxonomy

OUTPUTS.....

Dissemination

- Methods and emphasis varies with discipline
 - Journal vs Conference
 - Pure vs Applied
 - Research vs Application
- Authorship & Acknowledgements
 - Who goes on the paper?
 - Who is mentioned in the press release?
 - Do you acknowledge the technician?

Validation

- Increasing the value of data
- How to bring all the necessary information together to enable appropriate validation
- Increasingly difficult & expensive to achieve
- Need provenance and context
- Essential step otherwise just a collection of items

Plans and Provenance: Laying the Foundations

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.



If you can't describe what you are doing as a process, you don't know what you're doing.

W. Edwards Deming

Smart Tea Project

the Smart Tea Project



"I can go anywhere and its, like, this is
me and my data. Its all there, bang."

- Chris,
a real chemist, on using Smart Tea
instead of a paper lab book.

Making Tea

The Smart Tea project involves researchers from various fields within Chemistry and Computer Science. On the computer science team alone, we have researchers in semantic web information systems, grid computing, intelligent agents, web services, and human computer interaction.

In order for all of us to gain a better understanding of the chemists' lab experiences, and of the experimental design and execution process in particular, we *made tea* as a chemistry experiment. The experiment was lead by team member Graham Smith, a chemist and computer scientist.



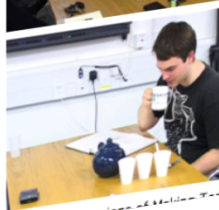
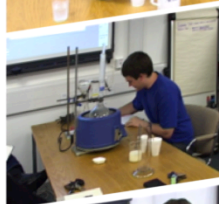
Smart Tea is
Smart Tea is
experimenta

Background

When chemists
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information is



Motivation



The Lab Aether

With the evolution of the Semantic Grid and Pervasive Computing (information and computers everywhere), it is possible to change our thinking about information away from the lab book to the *lab aether*.

The ancient concept of aether was of an invisible medium, all around us. In our concept of a lab aether, the aether is the invisible medium holding information being generated within the lab. As chemists build up an experiment, they release the data to the lab aether where it can be captured, reused and displayed in multiple contexts, from plan to publication.

We can think in terms of such an aether now because of research developments like web services, intelligent agents and the semantic grid. We use effective information interaction design to support scientists both populate data into the aether and grab it back as needed.

Part of the world wide [eScience Semantic Grid](#) effort is to get the data crafted by individual scientists out of the lab and onto the Grid, where it can be accessed, compared and processed within the global science community.

To that end, the Smart Tea Project is focussing on the experimental process itself in order to understand how the (usually hand written) information generated in the lab can be transformed into information accessible beyond the confines of a single experimental entry in a single paper-based lab book.

Chemistry and Tea: An Interesting History

[A Nice cup of Tea](#)

- George Orwell

[Chemists seek perfect cup of tea - for Orwell](#)

- London (Reuters)

[How to make the perfect cup of tea](#) (pdf download)

- The Royal Society of
Chemistry provide the
"definitive recipe for a cup
of tea"

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Press Release 10-077

Scientists Seeking NSF Funding Will Soon Be Required to Submit Data Management Plans

Government-wide emphasis on community access to data supports substantive push toward more open sharing of research data

May 10, 2010

If you have a plan then make use of it!

Just like the UK COSHH safety plans are ideal basis for driving an Electronic Laboratory Notebook

With a little extra work a plan becomes a useful way to provide context for the digital record

COSHH

Leverage off things we already have to do – “We have a cunning plan”

COSHH ASSESSMENT FORM			
			Record No.
SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD
Water	Liquid	1000ml	None
Dextrose	Solids	<20g	possible irritation to eyes and skin
Caffeine	Solids (bean)	<1g	Harmful if swallowed, induce vomiting.
Milk	Liquid	<100ml	No particular hazards
NATURE OF PROCESS liquid extraction of caffeine, followed by combination with dextrose to produce a sweet drink			
Is there a less hazardous substance? No If so, why not use it?			
CONTROL MEASURES REQUIRED (Local exhaust ventilation, personal protection, etc.) No specific measure required			



The fully semantic ELN - everything is linked!
Processes, materials and data

PLAN is a key ingredient to efficient and safe working

To Do
List

Plan

Process
Record

Ingredient List	
Fluorinated biphenyl	0.9 g
Br11OCB	1.59 g
Potassium Carbonate	2.07 g
Butanone	40 ml

Dissolve 4-fluorinated biphenyl in butanone

Add K₂CO₃ powder

Heat at reflux for 1.5 hours

Cool and add Br11OCB

Heat at reflux until completion

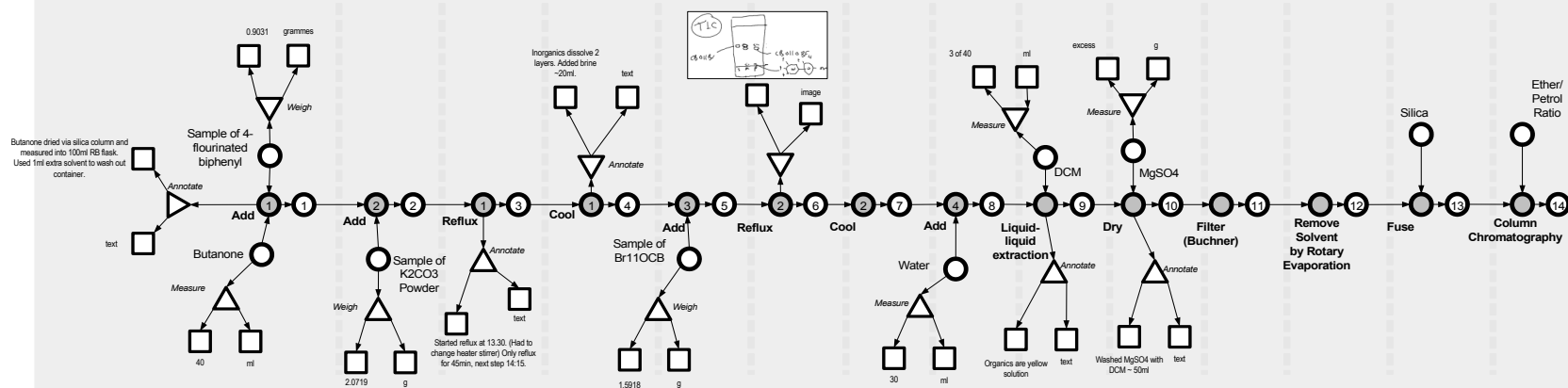
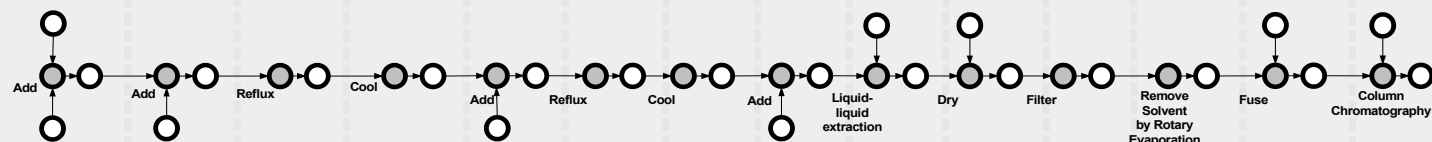
Cool and add water (30ml)

Extract with DCM (3x40ml)

Combine organics, dry over MgSO₄ & filter

Remove solvent in vacuo

Fuse compound to silica & column in ether/petrol



Key	
Process	○
Input	○○
Literal	□
Observation	▽

Observation Types	
weight - grammes	
measure - ml, drops	
annotate - text	
temperature - K, °C	

Future Questions	
Whether to have many subclasses of processes or fewer with annotations	
How to depict destructive processes	
How to depict taking lots of samples	
What is the observation/process boundary? e.g. MRI scan	

Combechem
30 January 2004
gvh, hrm, gms

Discussions – Is the tea room still the ‘heart’ of the department

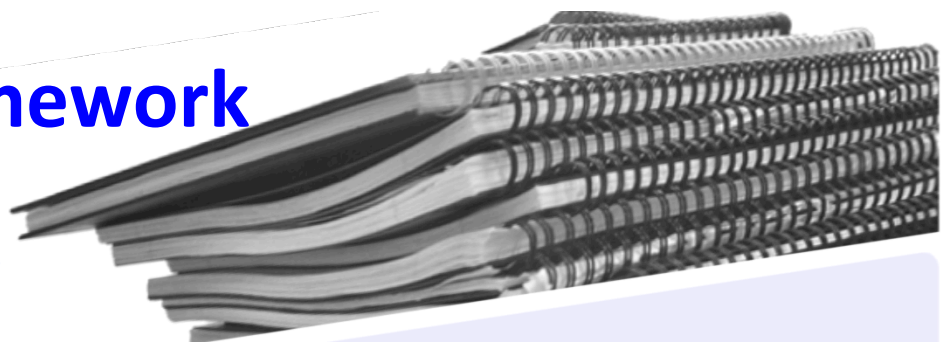


Growing need for the
global (virtual)
equivalent of the
“Tea Room”

Social Space? Space for Discussions?
Time for discussions?

Smart Research Framework

My Lab Notebook



Introduction

Introduction

Software Overview

Partners

Vision

SRF Software

LabTrove

Plan3

The SRF project
a shared virtual
management.

Providing tools to
meet the need
responsibility, co
use of
projects
mental a



06/07/2012

LabTrove

"preserving the record"

© flickr.com/julia_manzerova

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JISC CNI Conference

our experiment

Pictet-Spengler route to Praziquantel

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

17th March 2012 10:07:00

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

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- March 2012 (0)
- February 2012 (0)
- August 2011 (0)
- July 2011 (0)
- June 2011 (0)
- May 2011 (0)

Sections

- Experiments (0)

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

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

unreadable text · retweet · favorite

Transformation of plasmid JRH4712/66 into BW25141 by electroporation

11th December 2006 @ 14:31

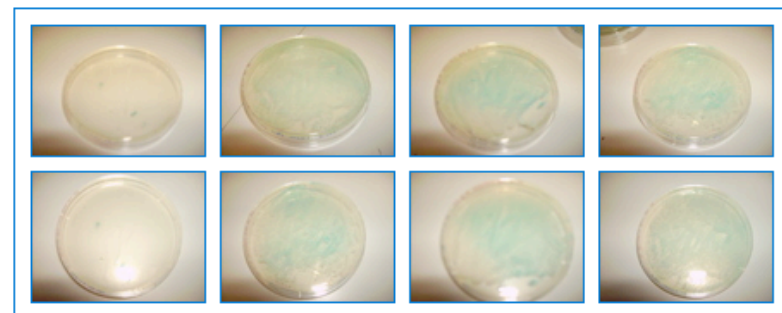
Transformations were set up according to the following protocol: LB Ampicillin arabinose plates and SOC medium were warmed to 37 °C briefly before the arabinose plates were spread with X-glu (80 µL, 1:1 X-glu and LB) and allowed to continue warming.

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 µL	7.5 µL	7.5 µL	10.5 µL	10 µL
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)

Mutagenesis of plasmid p042 via Taq and GenemorphI

9th January 2007 @ 14:34

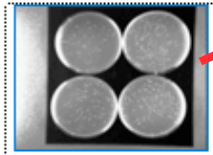
Lab Book Ref: jrh4712-78

Mutagenic PCR reactions were set up according to the following:

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

*GoTaq=1 µL stock + 3 µL water.

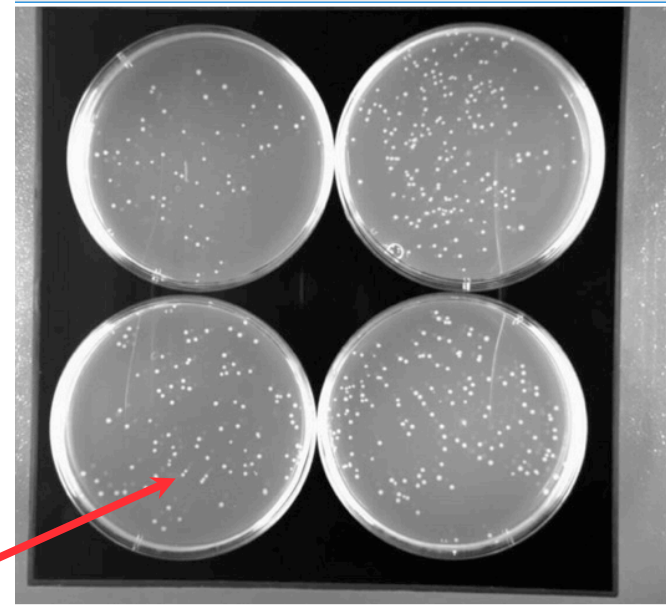
The reactions were run on program MUTAGG for 30 cycles. 5 µL product was run on a 1% normal agarose analytical gel. Taq mutagenesis had failed, Genemorph and +ve ctrl had worked. -ve control was correct.



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

[<< Previous Page](#)

[Next Page >>](#)



Core of Self describing data

- Store of data that can be viewed and manipulated in different ways
- User interfaces to suite user and occasion

He is charged with expressing contempt
for meta-data

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 no 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 emulsion separation. and turn porphyrin protonated green.
- much better behavior now....lovely shade of green too.



protonated porphyrin with 2M HCL

- HCL reextracted with 100ml CHCl₃.
- fluffily 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



27-11-08 (2)

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

Experiment Name

[Preparation Of Fulleropyrrolid](#)

[Alcohol:-Planning And Safety \(E](#)

[Preparation Of N-Glycine](#)

[\(amino-Ethoxy-Ethanol\) Tert](#)

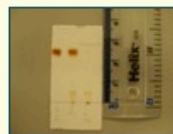
[Butyl Acetate \(4\)](#)

[Preparation Of P-tert Butyl](#)

[\(bis\(cyanomethoxy\)dihydroxy](#)

[Calix \(2\)](#)

[Preparation Of Mono Para Meth](#)



What Spotted (L-R):-starting material, mixed spot, reaction mixture

Spot (no. from bottom)	Height (mm)	Rf	Visible	Short Wave UV	Long Wave UV	Dip Type	Dip Result	Inference
Solvent Front	28mm	1	N/A	N/A	N/A	N/A	N/A	N/A
3	26mm	0.93	yes	N/A	orange	n/a	n/a	Starting material MeOTPP
2	10mm	0.36	yes VV faint (not on Photo present only in mix and reation)	n/a	Blue	n/a	n/a	decomposition?/contaminat?
1	6mm	0.21	yes	n/a	orange	n/a	n/a	product.

[1,4-Benzoquinone \(1\)](#)

[5-4-Methyl Benzoate](#)

[10,15,20-tri Phenyl Porphyrin](#)

(4)

**Diversity
and
Disability**

Impact on researchers

- Higher Quality Record
- Easier Collaboration
- Improved planning
- Improved discussions
- Efficiency gain in production of presentations/reports
- Change the nature of Professor/Student interactions

Open Notebook Science

- Not always the way to work!
 - IPR, Commercial, long term projects, recognition issues, etc
- But.....
 - Makes connection much easier if the data and processes are “Open”
 - Use of ChemSpider, GHS Data
 - Linked-Data ideal

Praziquantel – Open Science

Improved Synthesis of an Important Drug via Student Collaboration

Praziquantel Project

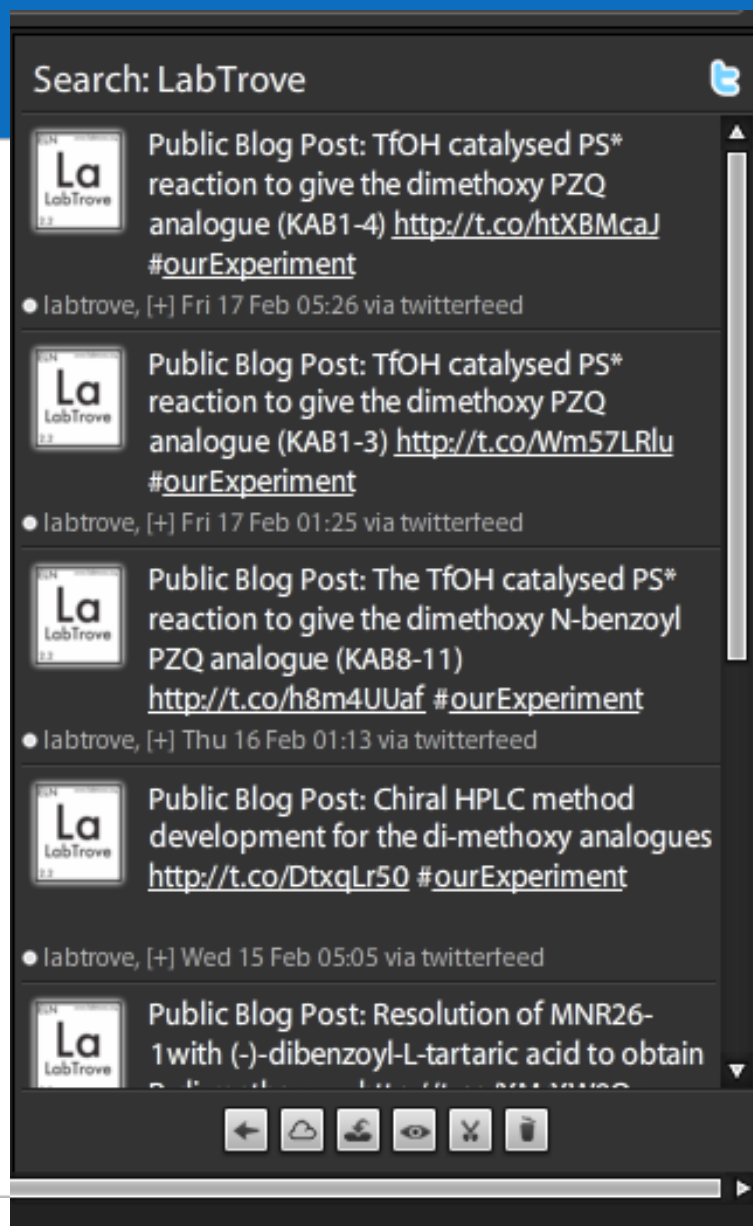
- [Introduction](#)
- [Project Updates](#)
- [Project Discussion](#)
- [ALTC links](#)

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](#)



Pictet-Spengler route to Praziquantel

Synthesis of intermediates and derivatives of PZQ

our experiment
alpha

Older Posts >>

Search

Archives

February 2012 (18)
January 2012 (27)
December 2011 (7)

TfOH catalysed partial PS* reactions to give the enediamide intermediates of PZQ and the N-benzoyl analogue (KAB13-2 & KAB17-1)

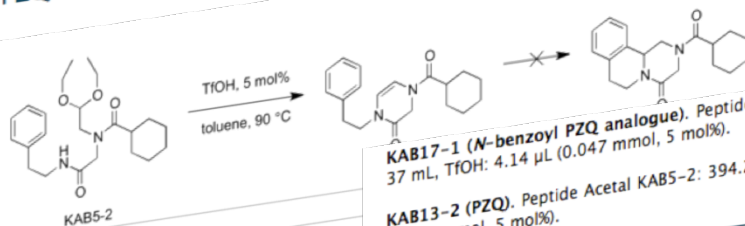
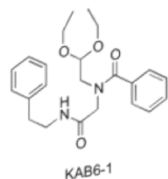
21st February 2012 @ 20:5

PS = Pictet-Spengler

START: 22/02/12
FINISH:

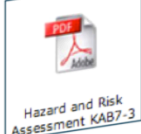
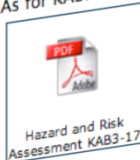
Background

Reducing the catalyst load



Hazard and Risk Assessment

As for KAB7-3 and KAB3-17.



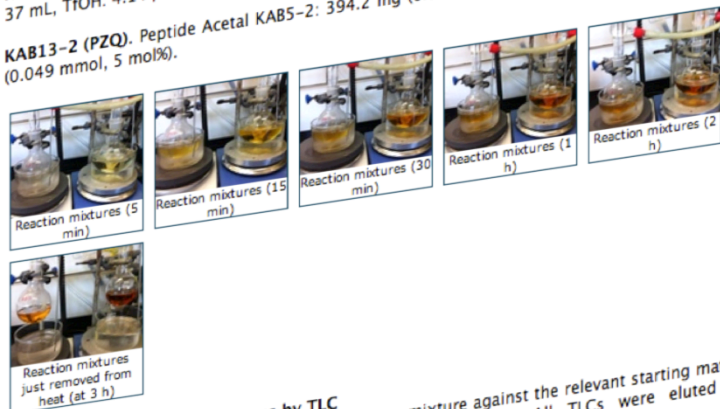
Previous Related Experiments

TfOH catalysed PS* reactions to give the dimer
TfOH catalysed PS* reaction to give PZQ (KAB
TfOH catalysed PS* reaction to give the N-benzoyl
Preparation of the PZQ peptide acetal Ugi-intermediate
Preparation of the N-benzoyl PZQ analogue U

Following Experiments

Procedure

The peptide acetal Ugi-intermediate starting
of TfOH at rt. The mixture was immediately
heated. The reaction progress was monitored



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 KMnO₄.



06/07/2012

JISC Online Conference

SHOW OPEN NOTEBOOKS



Welcome to the e-malaria Project!

Project Update

The project isn't currently being supported at the moment - but we hope to return soon with new funding and a bigger and better project website.



Home

CCDC

Lifecyc

e-Malaria

Backgr

Southa

School:

eScien

Publica



Molecules - My Molecules

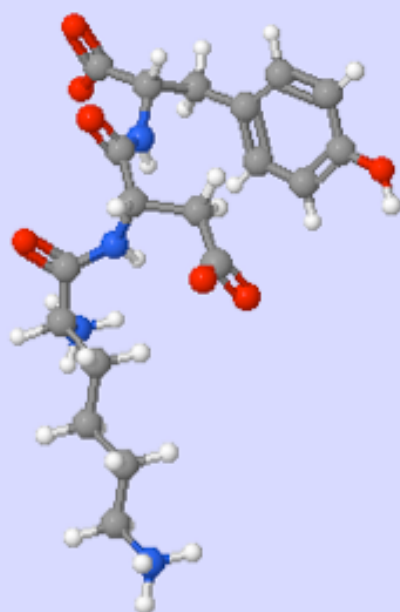
[Insert Molecule](#)

Id	Name	Smile	Image	Status	Jobs	Tools
----	------	-------	-------	--------	------	-------

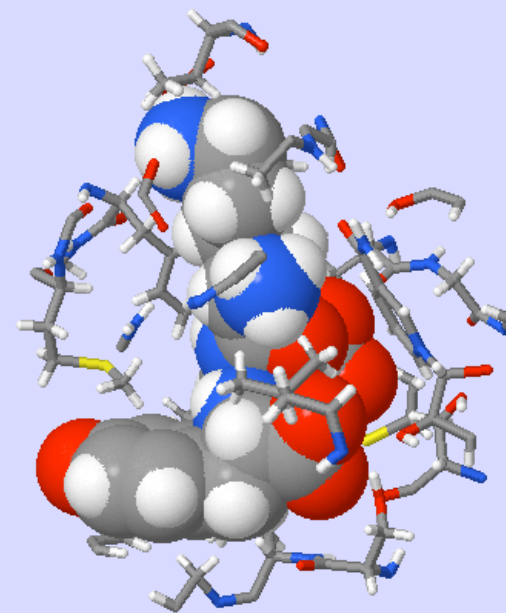
Sort By

available at this time.

se. As resistance to existing drugs grows ar



Jmol



Malaria

[Introduction](#)

[Symptoms](#)

[Treatments](#)

[Prevention](#)

[Target](#)

Some amino acids

Threonine thr t

Tryptophan trp w

Tyrosine tyr y

Valine val v

Methionine met m

Malaria

[Introduction](#)

[Symptoms](#)

[Treatments](#)

[Prevention](#)

[Target](#)

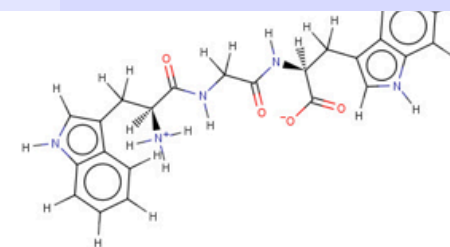
Chemistry

[Bonding](#)

[Hydrophobicity](#)

[Structure](#)

[Proteins](#)



06/07/2012

JISC CNI Content

Welcome to the e-malaria Project!
Project Update

The project isn't currently being supported at the moment - but we hope to return soon with new funding and a bigger and better project website.

Please feel free to look around the pages on the site as we can't make the interactive part available at the moment.

In the event of inquiry please contact the project manager.

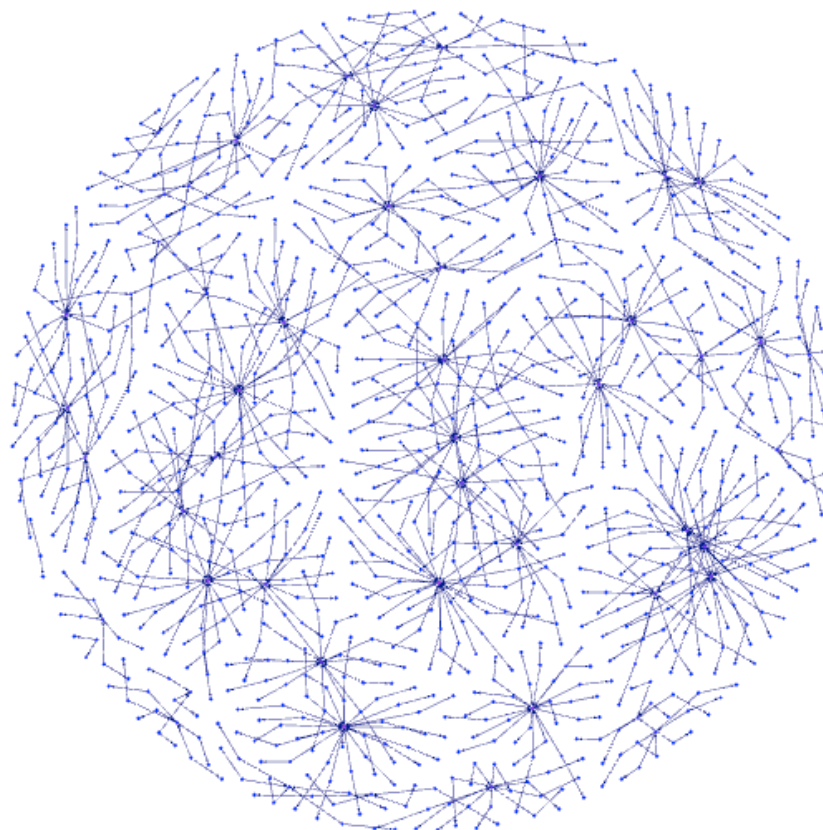
What's the problem?

Malaria kills over a million people a year, and the disease. As resistance to existing drugs grows, the need for new mosquito that need is increasing.

So what has this got to do with you?

Home
CCDC
Lifecycle
e-Malaria Project
Background
Southampton
Schools
eScience
Publications
Malaria
Introduction
Symptoms
Treatments
Prevention
Target

Shredded Tweet & eMalaria



Molecules - My Molecules

Sort By

Docking

Id	Name	Smile	Chemical Structure	3D	Score
58830	New Test 2	OC1CCC2(C1)C=CC=C2 ... InChI=1S/C9H12O/c10-8-3-6-9(7-8)4-1-2-5-9/h1-2,4-5,8,10H,3,6-7H2...		3D	1/1 (31.60:31.60)
58829	New Test	C1=CC2=CC=CC=C2C=C1 ... InChI=1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H...		3D	1/1 (27.32:27.32)
58828	CCCCccccccc	...		3D	0/0 (0.00:0.00)
58783	name	...		Error	-
58782	name	...		Error	-

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Hydrophilicity

Plasmepsin II (1LF2) scored 62.76 <http://emalaria.soton.ac.uk/77772>

Plasmepsin II (1LF2) scored 59.05 <http://emalaria.soton.ac.uk/77773>

Plasmepsin II (1LF2) scored 51.68 <http://emalaria.soton.ac.uk/77774>

Plasmepsin II (1LF2) scored 60.54 <http://emalaria.soton.ac.uk/77775>

Plasmepsin II (1LF2) scored 59.38 <http://emalaria.soton.ac.uk/77777>

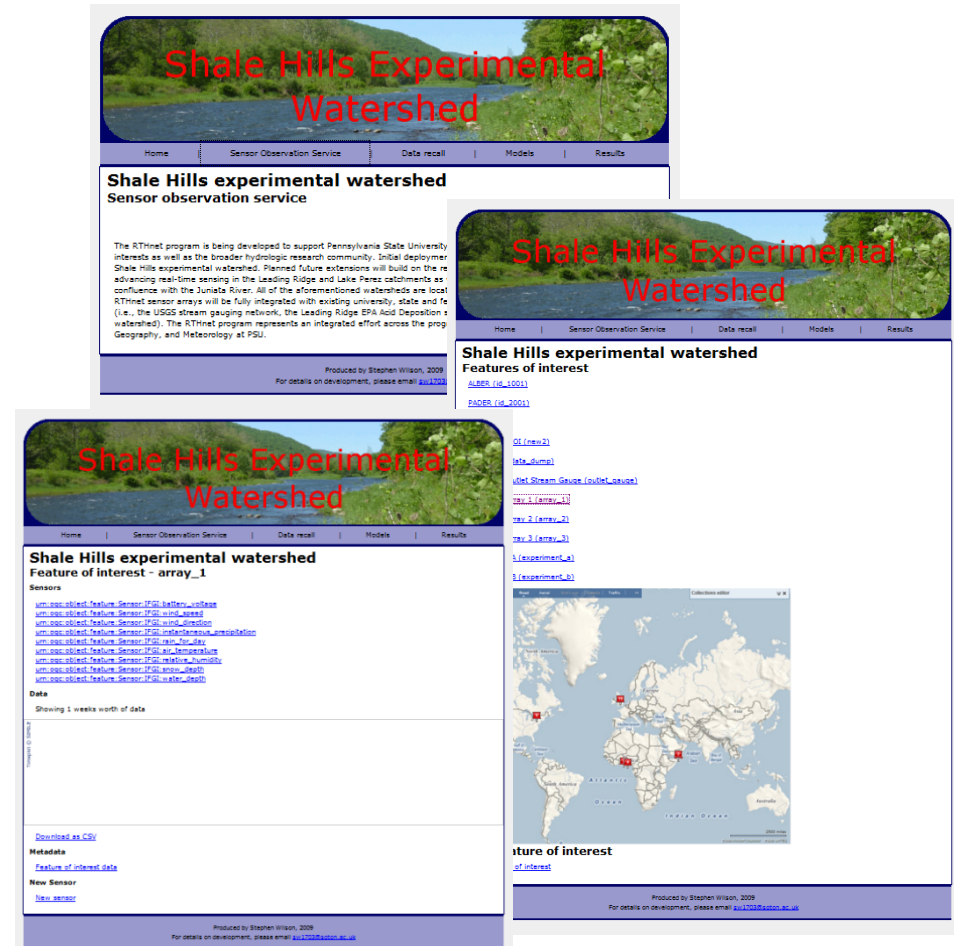
Plasmepsin II (1LF2) scored 70.65 <http://emalaria.soton.ac.uk/77780>

Plasmepsin II (1LF2) scored 58.92 <http://emalaria.soton.ac.uk/77781>

Twitter

Web Interface

- Provide user access to the SOS
- Provides mechanisms to retrieve data and metadata of both the sensors and the features of interest
- Data plotted using the Simile TimePlot software

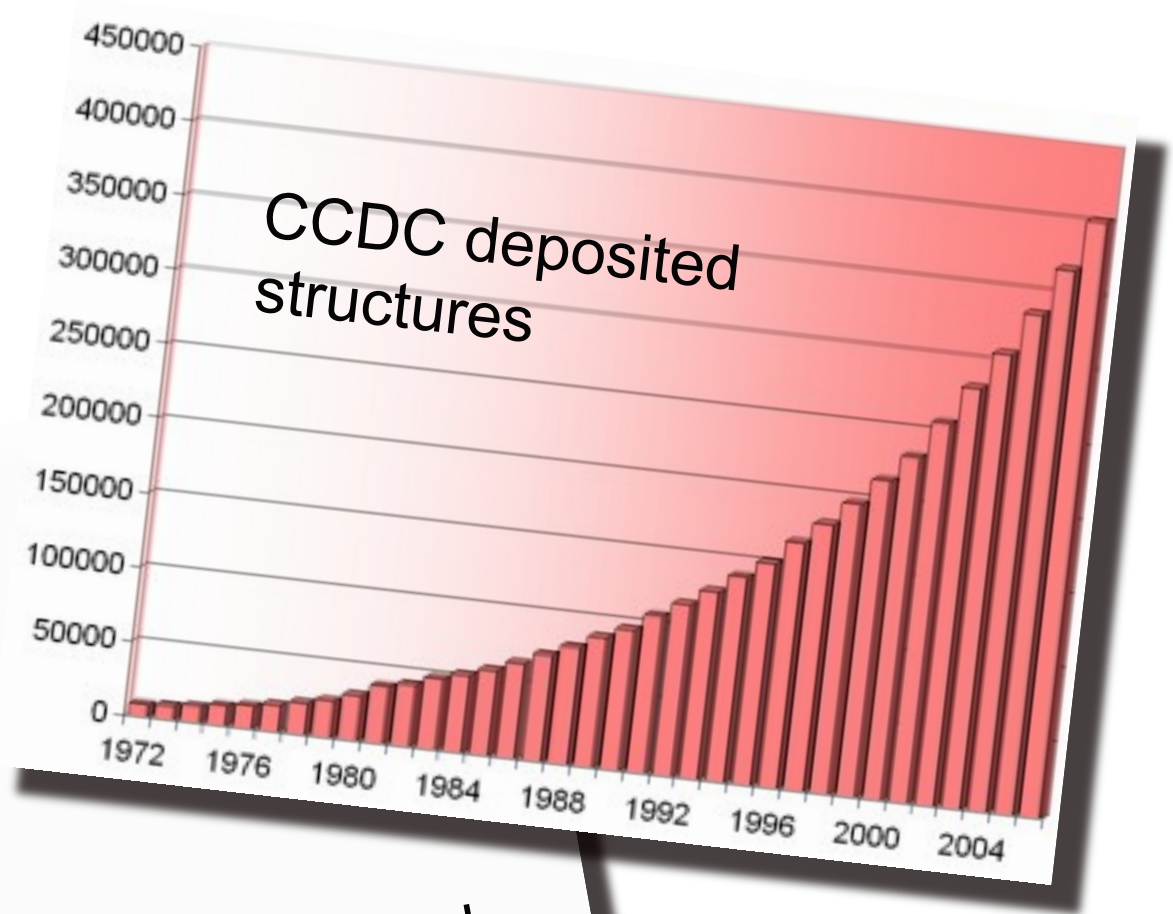
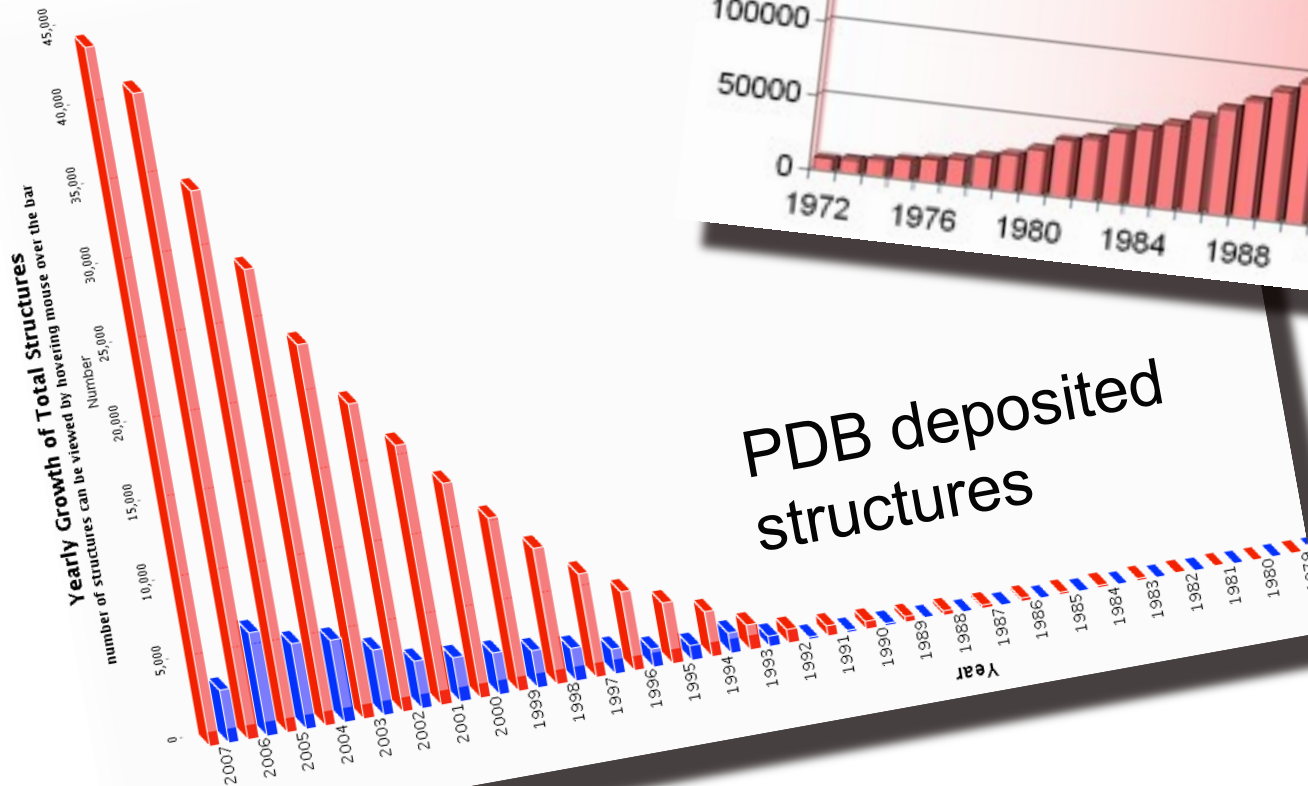


DATA EXPLOSION

CRYSTALLOGRAPHY E-CRYSTALS

The Data Explosion

Exponential growth



PDB deposited structures

The future
overwhelms the
past,
but the past
must not be lost

Unavailable Information

- Not just lots of data but why are many of the structures unpublished so certainly unavailable?
- The E-Crystals and E-Bank Project looked at how to address this issue
- Is making data available the same as depositing a copy with someone else?

Sample Originator: Esther Rousay^a and Jeremy G. Frey^a.

Data Collection: Simon J. Coles^a

Structure Determination: Simon J. Coles^a and Michael B. Hursthouse^a.

University of Southampton

eCrystals

Home | About | Browse by Year | Browse by People

Back

You are viewing an HTML version of this document. To see the underlying XML use your web browsers "View Page Source" option.

6,7,9,10,12,13,15,16-Octahydro-benzo-1,4,7,10,13-pentaoxacyclopentadecin

C₁₄H₂₀O₅

InChI=1/C14H20O5

Identification Number

Controlled Keyword

Date Created

Deposit

Deposit

Depositor

Structure alr

project.

Data colle

Chemical fo

Identifier: <http://>

Creator: Rou

Creator: Frey

Creator: Cole

Creator: Hur

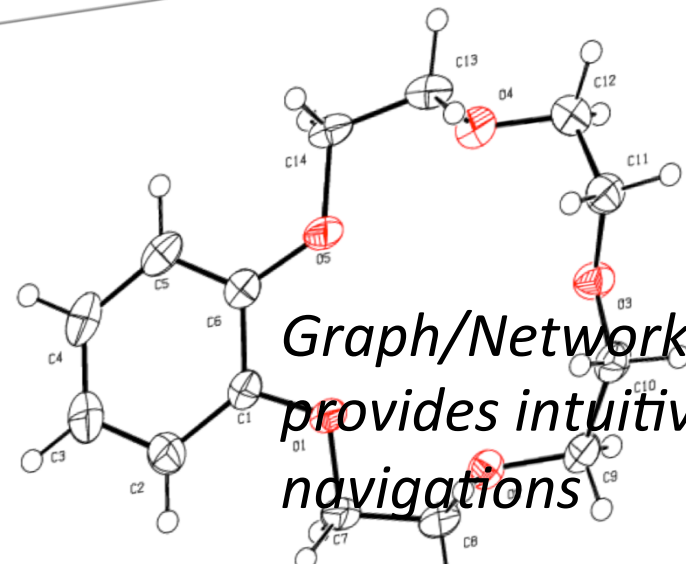
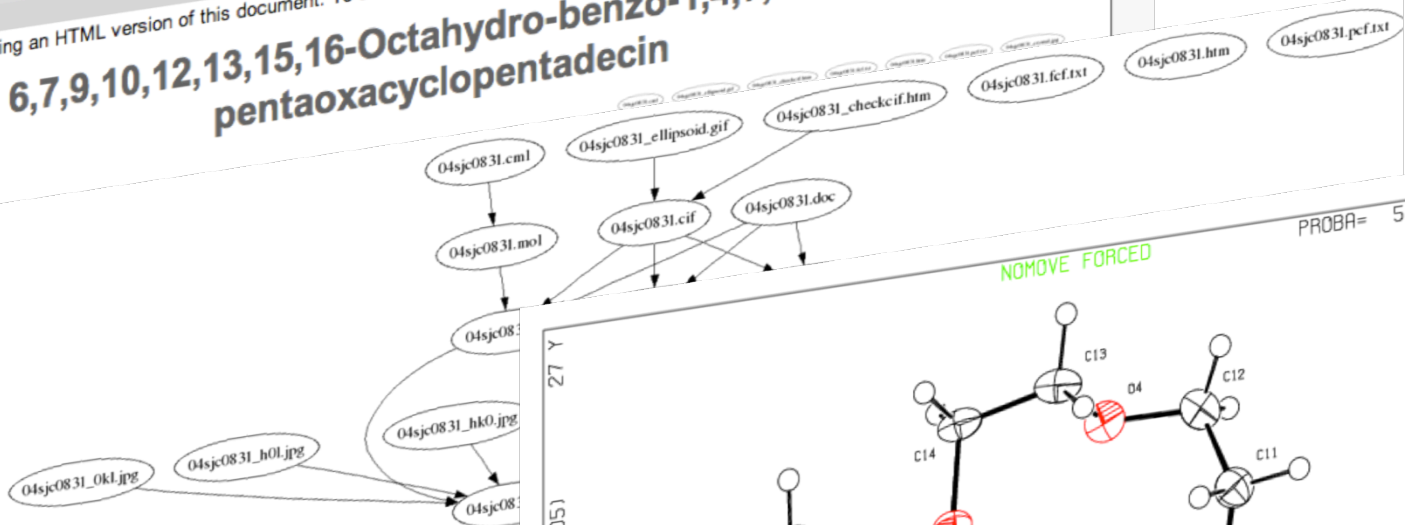
Date: 200

Stages (10)

Stage:

1 [plan.rdf](#)

2 [plan.rdf](#)



Graph/Network
provides intuitive
navigations

06/07/2012

JISC CNI Conf

27 Y
27 14:31:25 2005 - (120405)

PROBA= 50

*It is not necessary to change.
Survival is not mandatory.*
W. Edwards Deming

START @HOME PUBLICATION@SOURCE



Reproducible Papers

literateprogramming.com

Literate Programming

Quotes

- Literate Programming
- Software Documentation
- Design Documentation
- Agile Documentation
- Source Code Comments
- Software Aging
- Quotes - Printer Friendly

Category

- CWEB
- Articles
- Tools
- Links

Community

- Feedback

Donald Knuth. "Literate Programming (1984)" in Literate Programming. CSLI, 1992, pg. 99.

I believe that the time is ripe for significantly better documentation of programs, and that we can best achieve this by considering programs to be works of literature. Hence, my title: "Literate Programming."

Let us change our traditional attitude to the construction of programs: Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do.

The practitioner of main concern is with the thesaurus in hand, each variable means because its concept understanding, using each other.

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

INSTITUT FÜR STATISTIK - COMPUTATIONALE STATISTIK
PROF. FRIEDRICH LEISCH

Home | AG Computationale Statistik | Institut für Statistik | LMU

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- Statistical computing
- Software

PUBLICATIONS

- Books
- Papers
- Reports
- Presentations

LINKS

- R
- Bioconductor
- Journal "Comp. Statistics"
- Munich R Courses
- Herbstschule 2008

The Sweave Homepage

What is Sweave?

Sweave is a tool that allows to embed the [R](#) code for complete data analyses in latex documents. The purpose is to create dynamic reports, which can be updated automatically if data or analysis change. Instead of inserting a prefabricated graph or table into the report, the master document contains the R code necessary to obtain it. When run through R, all data analysis output (tables, graphs, etc.) is created on the fly and inserted into a final latex document. The report can be automatically updated if data or analysis change, which allows for truly reproducible research.

Where can I get it?

The Sweave software itself is part of every [R installation](#), see `help("Sweave", package="utils")`

to get started. This page features additional material that does not ship with standard R, like papers and additional examples.

How do I cite Sweave?

To cite Sweave please use the paper describing the first version:

R/LISP Papers

Quantity

Names

Symbol

Value

Units

Prov

```
P <- read("http://eprints.soton.ac.uk/frey/reproducible.  
computable.paper")
```

Summary(p)

The rate constant for the OH reactions.....

Abstract(p) vs p\$Abstract {First abstracts the paper, second gives the
papers' abstract}

p\$Title

OH Rate constants for Atmospheric Chemistry and Combustion

Print(p\$Text); variables <- p\$Quantities

Graph <- p\$Graphs or to access the data in the graph p\$Graphs\$Table\$Quantities

Context(P)

$\Delta_f H(\text{OH}) =$

Context(P) <- New.Context(new_thermodynamic_data)

p1 <- Run(p) ; run with new context : value of $\Delta_f H(\text{OH})$

Warninh:you do not have the resources to re-run this paper....

Diff <- p - p1 ; what conclusions change

Frey & DeRoure

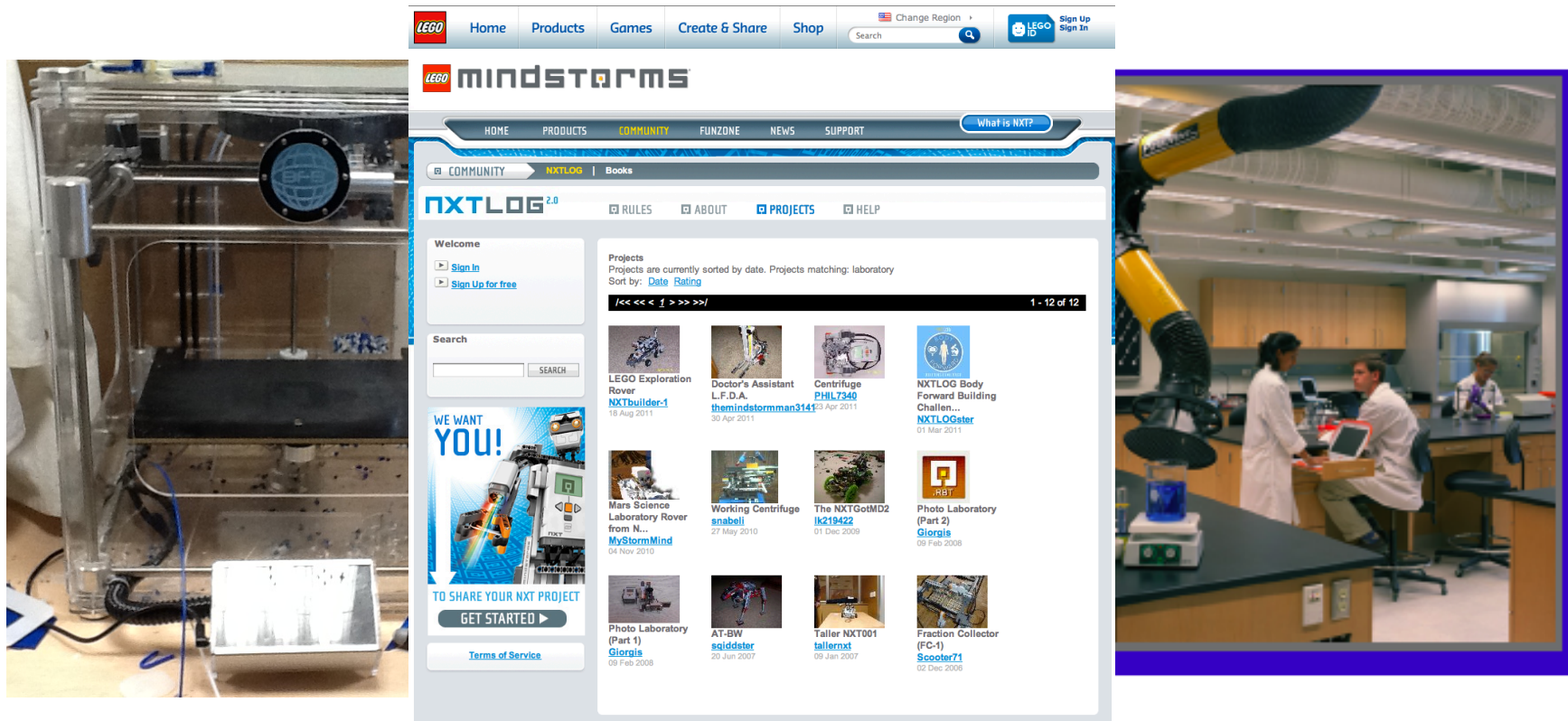
Stockholm

4t Paradigm Next Step

meeting

4 Dec 2011

Change in the whole way we design and build



3D Printers

Shared Space?

NATURE | NEWS FEATURE

Science in three dimensions: The print revolution

Three-dimensional printers are opening up new worlds to research.

Nicola Jones

04 July 2012



Research labs use many types of 3D printers to construct everything from fossil replicas to tissues of beating heart cells. Arthur Olson's team at the Scripps Research Institute in La Jolla, California, produces models of molecules; some are shown here partway through the printing process.

ADAM GARDNER, MOLECULAR GRAPHICS LAB AT TSRI

Archiving of data

- Experiments are often repeated
 - Data stored locally on a computer and can't be found
 - Handwriting can't be read
 - Laboratory notebooks lost or damaged
 - Correct data not recorded first time round



<http://www.ecs.soton.ac.uk/regenesis/pictures>

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*

Thanks

- UK e-Science Programme
- RCUK, EPSRC, JISC, BBSRC, HEFCE, Microsoft & IBM, for funding
- Southampton Colleagues and Students from Chemistry, Electronics & Computer Science, Engineering, Mathematics, iSolutions and the Library
- Colleagues at UKOLN, STFC, University of Reading
- Colleagues from Penn State, Cornell, PNNL, UNSW, USyd



Thank you for listening

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