

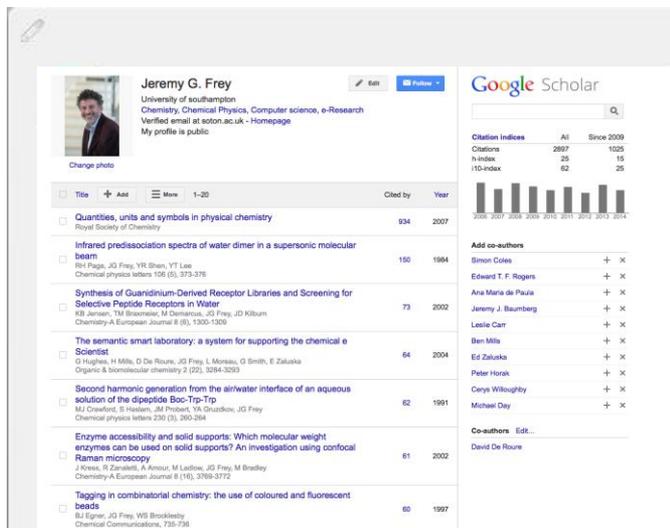


Science Ajar?

From Open Access to Intelligently Accessible Data in Open Notebooks

Jeremy G. Frey
University of Southampton

A Chemist's Digital Aura



Jeremy G. Frey
University of southampton
Chemistry, Chemical Physics, Computer science, e-Research
Verified email at soton.ac.uk - Homepage
My profile is public

Citation indices All Since 2009

Index	All	Since 2009
Citations	2997	1025
h-index	25	15
i10-index	62	25

Quantities, units and symbols in physical chemistry
Royal Society of Chemistry
934 2007

Infrared predissociation spectra of water dimer in a supersonic molecular beam
Ri Page, JG Frey, YH Shen, YF Lee
Chemical physics letters 158 (5), 373-376

Synthesis of Guanidinium-Derived Receptor Libraries and Screening for Selective Peptide Receptors in Water
KJ Jensen, TM Brorsson, M Damsgaard, JG Frey, JD Kilburn
Chemistry-A European Journal 8 (9), 1300-1309

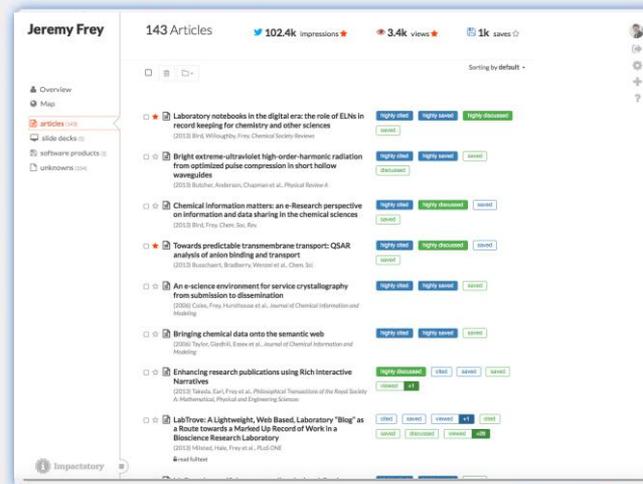
The semantic smart laboratory: a system for supporting the chemical e Scientist
G Hughes, M Mills, D De Roure, JG Frey, L Mossak, G Smith, E Zaluska
Organic & biomolecular chemistry 2 (22), 3284-3293

Second harmonic generation from the air/water interface of an aqueous solution of the dipeptide Boc-Trip
KJ Crawford, B Hoadley, JM Probst, VA Guskow, JG Frey
Chemical physics letters 230 (3), 260-264

Enzyme accessibility and solid supports: Which molecular weight enzymes can be used on solid supports? An investigation using confocal Raman microscopy
J Pines, R Zarnitski, A Anwar, M Ladlow, JG Frey, M Bradley
Chemistry-A European Journal 8 (16), 3769-3772

Tagging in combinatorial chemistry: the use of coloured and fluorescent beads
M Eigner, JG Frey, WS Brockley
Chemical Communications, 735-738

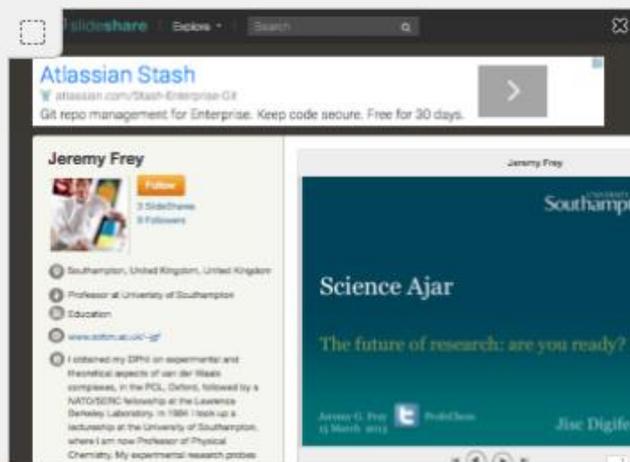
Jeremy G. Frey – Google Scholar Citations



Jeremy Frey
143 Articles
102.4k impressions
3.4k views
1k saves

- Laboratory notebooks in the digital era: the role of ELNs in record keeping for chemistry and other sciences**
(2013) Bird, Willoughby Frey, Chemical Society Review
- Bright extreme-ultraviolet high-order-harmonic radiation from optimized pulse compression in short hollow waveguides**
(2013) Buchert, Andorjan, Chapman et al., Physical Review A
- Chemical information matters: an e-Research perspective on information and data sharing in the chemical sciences**
(2013) Bird, Frey, Chem Soc Rev
- Towards predictable transmembrane transport: QSAR analysis of anion binding and transport**
(2013) Buschert, Bradberry, Wood et al., Chem Sci
- An e-science environment for service crystallography from submission to dissemination**
(2010) Cole, Frey, Nordmann et al., Journal of Chemical Information and Modeling
- Bringing chemical data onto the semantic web**
(2004) Taylor, Gorbil, Essex et al., Journal of Chemical Information and Modeling
- Enhancing research publications using Rich Interactive Narratives**
(2013) Tavares, Earl, Frey et al., Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences
- LabTrove: A Lightweight, Web Based, Laboratory "Blog" as a Route towards a Marked-Up Record of Work in a Bioscience Research Laboratory**
(2012) Wood, New, Frey, Proc RSC

Impactstory: Jeremy Frey



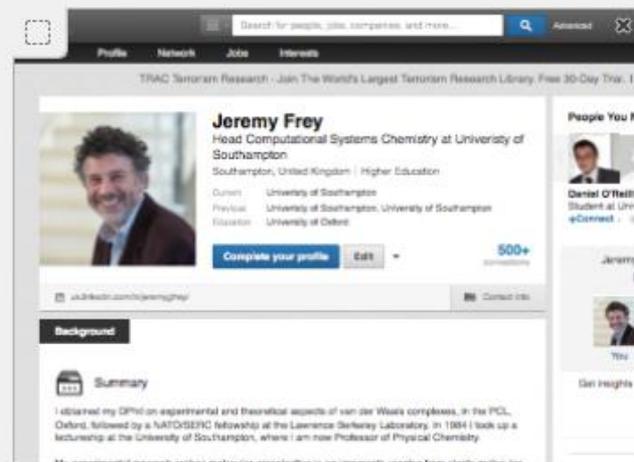
Atlassian Stash
atlassian.com/Stack-Enterprise-Git
Git repo management for Enterprise. Keep code secure. Free for 30 days.

Jeremy Frey
3 SlideShares
8 Followers

- Southampton, United Kingdom, United Kingdom
- Professor at University of Southampton
- Education
- www.soton.ac.uk/~jgf

I obtained my DPhil on experimental and theoretical aspects of van der Waals complexes, in the PCL, Oxford, followed by a NATO/DFRC fellowship at the Lawrence Berkeley Laboratory. In 1994 I took up a lectureship at the University of Southampton, where I am now Professor of Physical Chemistry. My experimental research probes

Jeremy Frey, Professor at Univeristy of south...



Jeremy Frey
Head Computational Systems Chemistry at University of Southampton
Southampton, United Kingdom | Higher Education

Current: University of Southampton
Previous: University of Southampton, University of Southampton
Education: University of Oxford

Background

Summary

I obtained my DPhil on experimental and theoretical aspects of van der Waals complexes, in the PCL, Oxford, followed by a NATO/DFRC fellowship at the Lawrence Berkeley Laboratory. In 1994 I took up a lectureship at the University of Southampton, where I am now Professor of Physical Chemistry. My experimental research probes molecular organization in environments ranging from single molecules

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A Chemist's Digital Aura



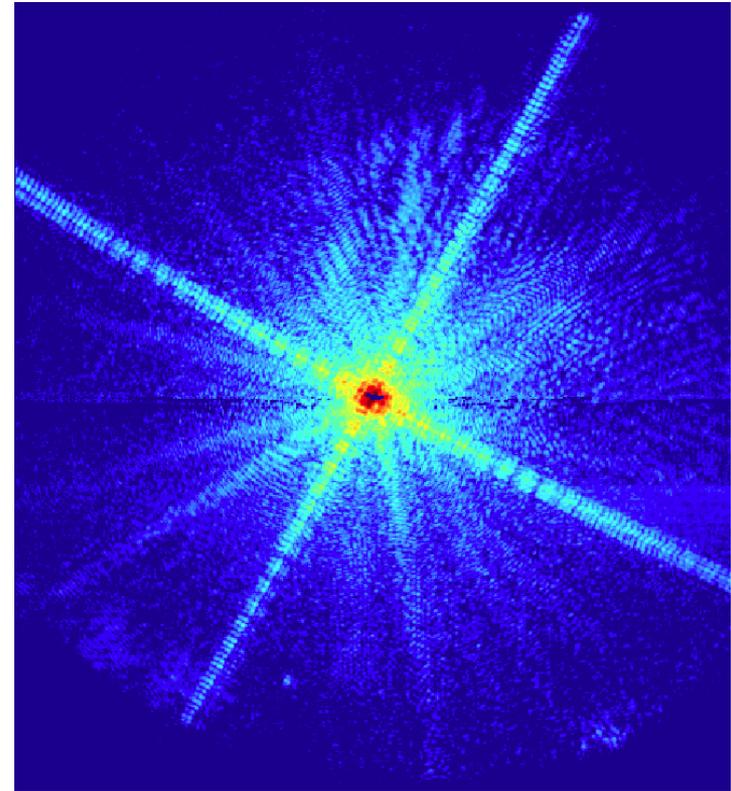
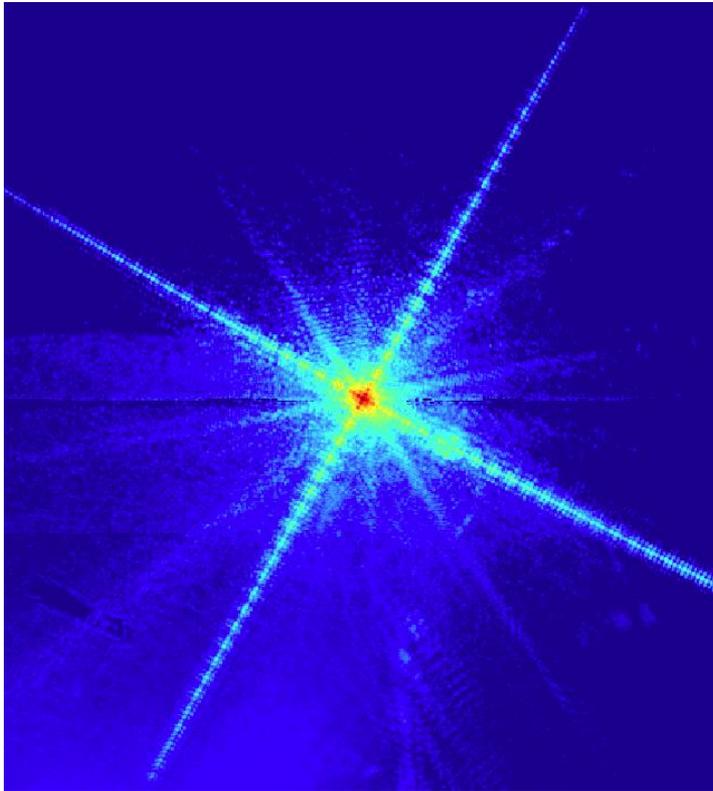
<http://mosaically.com/PhotoMosaic/3289771f-0bf3-49bf-bc8a-1810167096ff>

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



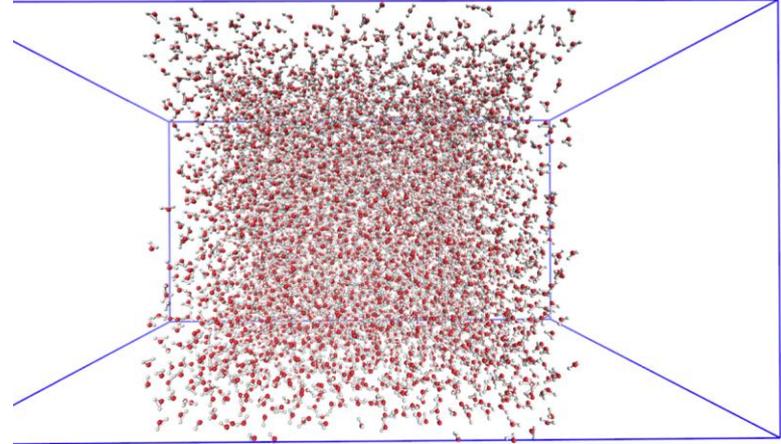
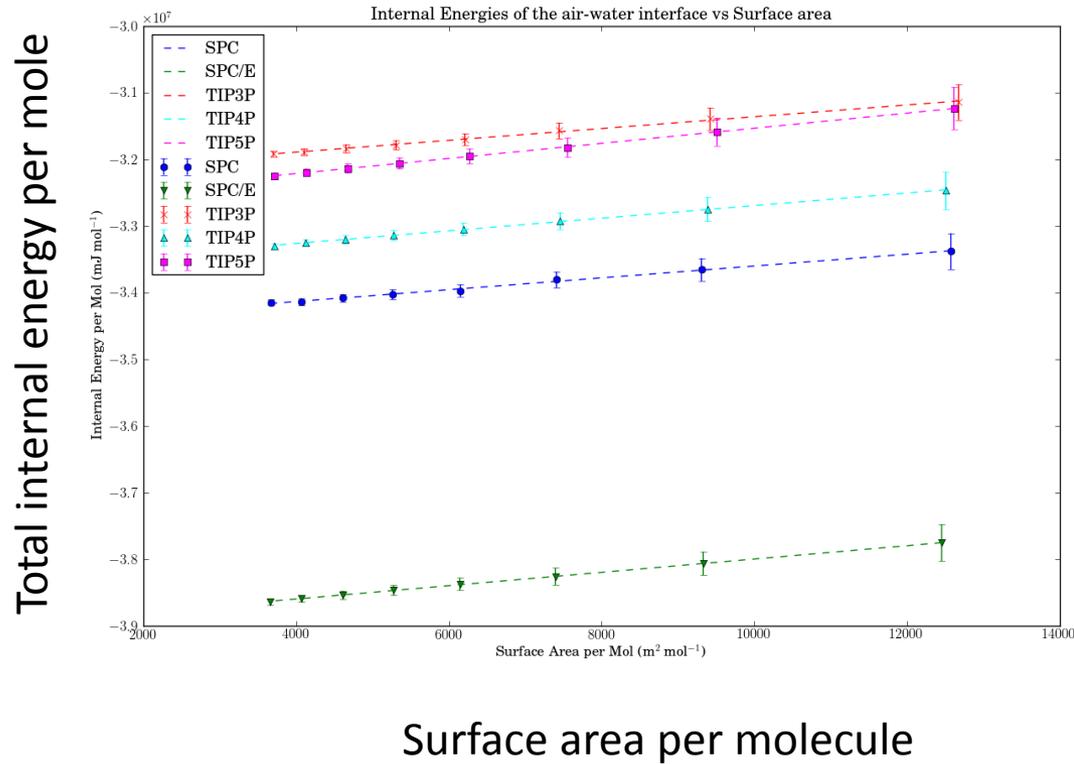
Reducing and Managing Uncertainty

Coherent diffraction Imaging for lensless soft x-ray microscopy



Key is computational phase reconstruction, which using GPU, can be done in time comparable to the experimental acquisition time. GPU cluster will enable ensemble solution and thus estimate the uncertainty in the reconstructing, but would need on demand.

Air/Water slab MD simulation



Computational power now available means that sufficient accuracy and low uncertainty can be obtained for a whole series of small and large water slabs allowing the surface contribution to the total energy to be reliably “observed” and entropy contributions to surface tension derived.

Reducing Uncertainty

- What is already known?
- Who is doing what?
- How was a result obtained?
- Access to Data
- Integration of Data.
- *Provenance & Planning*



Intelligent (Open) Access to Data

The screenshot shows the Royal Society website page for the 'Science as an open enterprise Final report'. The page features a red header with the Royal Society logo and navigation links. The main content area includes a title, a date (21 June 2012), and several paragraphs of text. A central image shows a complex network diagram with red and blue lines. To the right, there is a 'Download' section with links for the final report, summary, EPUB and Kindle version, and references. A sidebar on the right contains a 'Share this page' section and a 'Science as an open enterprise' section with links to case studies, launch event, public meeting, and call for evidence.

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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
- 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

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.

<https://royalsociety.org/policy/projects/science-public-enterprise/Report/>



Confusion over open-data rules

The Public Library of Science's pioneering open-data mandate has prompted scientists to share more data online, but not everyone is complying with the regulation.

BY RICHARD VAN NOORDEN

The mantra of the nascent open-data movement — that scientists should share online all data underlying their findings — sounds simple. But it can be tough to achieve in practice. An informal audit of one of the movement's biggest proponents, the Public Library of Science (PLOS), shows that not everyone is complying with the publisher's pioneering open-data mandate, and hints at the challenges that journals can face in enforcing open-data goals.

The idea that the progress of research will be accelerated if others can easily and freely build on data sets is gaining currency. Last week the Bill & Melinda Gates Foundation in Seattle, Washington, announced that it would demand open data of the researchers it funds.

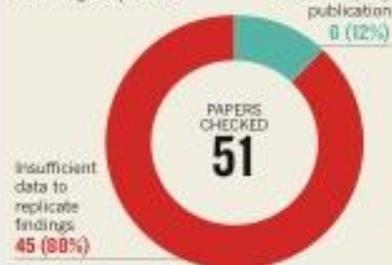
But whereas some research communities, such as geneticists and crystallographers, have long-established norms of open data, most funders and publishers (including *Nature*), mindful of researcher autonomy, merely exhort scientists to make their data open. Many surveys have found that scientists are worried about being scooped on future projects, or argue that they have signed agreements not to share their data.

So it was a step-change when in March PLOS made it a requirement that authors who publish in its journals share online all the data necessary to reproduce their studies. It was not

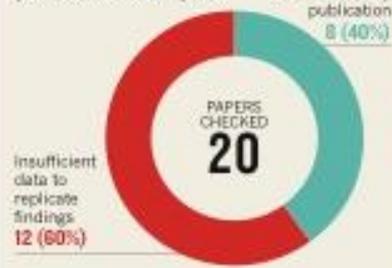
FREE THE DATA

In 2014, open-access publisher PLOS introduced a requirement that authors who publish in its journals make their underlying data freely available online. An informal audit of one type of population genetics study in one journal, *PLoS ONE*, shows that not everyone is complying — but the mandate is still a boon for the open-data movement.

2013-12, when PLOS encouraged open data



Since March 2014, after open-data mandate in place



job of external peer reviewers to check whether appropriate underlying data were available, he says. And although *PLoS ONE* was grateful for their help, "there is a learning curve here for all involved to understand what the data-sharing standards are for all disciplines and data types". He adds that once someone complains, the journal has a system for investigating papers that do not comply with its open-data requirement.

The research teams in question, nine of whom responded to the *Nature* news team's request for an explanation, provide an insight into why data sharing does not always happen in the first place (full data are available at go.nature.com/8ggob6). Some had forgotten to upload their data and promptly rectified the fault. Four teams said that the journal's editors and referees had never asked them to share the underlying genetics data, suggesting confusion over what the policy means.

Others aired wider — and common — objections to online data sharing. Even though they had chosen to publish with PLOS, some authors said that they wanted to hold back their data for future studies, or did not want to share the raw data unless they knew future users' intent.

Steve Simpson at the University of Exeter, UK, who reported work on Omani clownfish, said he was happy to share raw data privately with potential collaborators, but not to upload results from 400 individual fish that had taken great effort to collect. "The study is described so that it could be replicated by another exper-

SOURCE: TIM WAINES



<http://www.nature.com/news/confusion-over-publisher-s-pioneering-open-data-rules-1.16409>

Previous post

Energy outlook sees continuing dominance of fossil fuels



NATURE NEWS BLOG

Gates Foundation announces world's strongest policy on open access research

21 Nov 2014 | 18:39 GMT | Posted by [Richard Van Noorden](#) | Category: [Policy](#), [Publishing](#)

The Bill and Melinda Gates Foundation has announced the world's strongest policy in support of open research and open data. If strictly enforced, it would prevent Gates-funded researchers from publishing in well-known journals such as *Nature* and *Science*.

On 20 November, the medical charity, based in Seattle, Washington, [announced](#) that from January 2015, researchers it funds must make open their resulting papers and underlying data sets immediately upon publication — and must make that research available for commercial reuse. "We believe that published research resulting from our funding should be promptly and broadly disseminated," the foundation states. It says it will pay the necessary publication fees (which often amount to thousands of dollars per article).

<http://blogs.nature.com/news/2014/11/gates-foundation-announces-worlds-strongest-policy-on-open-access-research.html>



PHILOSOPHY

What we don't know

Michael Shermer enjoys a reminder that cutting-edge research is a step into the unknown.

At a press conference in 2002, Donald Rumsfeld, then US secretary of defence, used epistemology to explain US foreign entanglements and their unintended consequences. “There are known knowns; there are things we know we know. We also know there are known



Firestein introduces the concept of ignorance by contrasting the public's perception of science — as a systematic process — with a scientists' understanding that

MARTIN O'NEILL

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*“In theory, there is no difference between theory and practice.
But, in practice, there is.”*

Unknown (possibly Yogi Berra or Manfred Eigen)



Methods are as important as the data

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

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

E-mail this to a friend Printable version

'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 climate research institutions - is being intensely debated on the web. But what does it imply for climate science? Here, Mike Hulme and Jerome Ravetz say it shows that we need a more concerted effort to explain and engage the public in understanding the processes and practices of science and scientists.

As the repercussions of [ClimateGate](#) reverberate around the virtual community of global 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.



THE GREEN ROOM

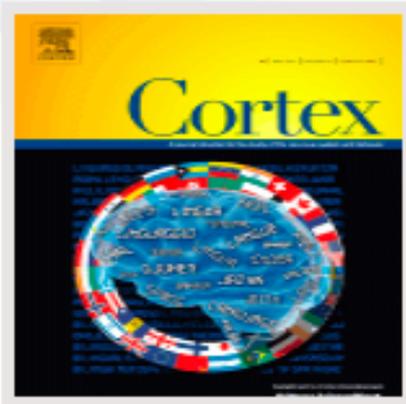
A weekly series of thought-provoking opinion pieces on environmental topics

Reviving Rio
The second Earth Summit holds the promise to cure the world's environmental ills

Your comments

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- Hailing the arrival of alien predators



8 May 2013  6 Comments

Journal Cortex launches Registered Reports



 Print or  PDF this page

Dr Chris Chambers and Professor Sergio Della Sala | Associate Editor and Editor-in-Chief of the Elsevier journal *Cortex*

On May 1st, *Cortex* launched a new innovation in scientific publishing called a Registered Report. Unlike conventional publishing models, Registered Reports split the review process into two stages. Initially, experimental methods and proposed analyses are pre-registered and reviewed before data are collected. Then, if peer reviews are favourable, we offer authors "in-principle acceptance" of their paper. This guarantees publication of their future results providing that they adhere precisely to their registered protocol. Once their experiment is complete, authors then resubmit their full manuscript for final consideration.

<http://editorsupdate.elsevier.com/short-communications/journal-cortex-launches-registered-reports/>



MARINE SCIENCE

Ocean observatory project hits rough water

Problems with data management challenge US effort to monitor seas in real time.

BY ALEXANDRA WITZE

From the waters off western North America to the seas surrounding Greenland, US oceanographers have nearly finished deploying hundreds of sensors, moorings, gliders and other equipment that make up an ambitious US\$386-million effort to establish the world's biggest interactive portal to the oceans. Through the Ocean Observatories Initiative (OOI), set for completion by May 2015, anyone could watch the climate changing in the North Pacific or an underwater volcano erupting in real time.

But even as the final instruments splash

into the sea, the project has hit a snag. After spending \$37 million to develop state-of-the-art software to manage live data, the OOI has terminated that contract — shifting responsibility for 'cyberinfrastructure' from the University of California, San Diego (UCSD), to a group based at Rutgers University in New Brunswick, New Jersey.

The shift is meant to help the OOI finish construction on time and on budget by next spring, and is likely to delay the start of data streaming by only a few months. Still, it is making some oceanographers anxious, given the project's broad scope. Data from its observatories are likely to dominate US oceanography for the

next 25 years — the OOI's planned lifetime.

The project, funded by the US National Science Foundation, is intended to be for the oceans what earthquake and volcano monitors are for the land: a way to allow real-time glimpses into the currents, marine life and chemistry in the deep sea. It will scrutinize a few select patches of ocean in exhaustive detail, using instruments attached to cables and on free-sailing gliders to measure temperature, salinity, chemistry and other key oceanographic parameters. The network's scattered locations include a cabled sea-floor observatory off the coast of Oregon; sets of instrumented moorings off the US east and west coasts; and

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<http://www.nature.com/news/ocean-observatory-project-hits-rough-water-1.16406>



<http://997waystobeagreatspeaker.com/2010/12/how-to-tell-a-story/>

*Skills we need are
story telling skills
not data mining
skills*

Clive Humby
DE/2014 Keynote



*“We have lots of information technology. We
just don’t have any information.”*

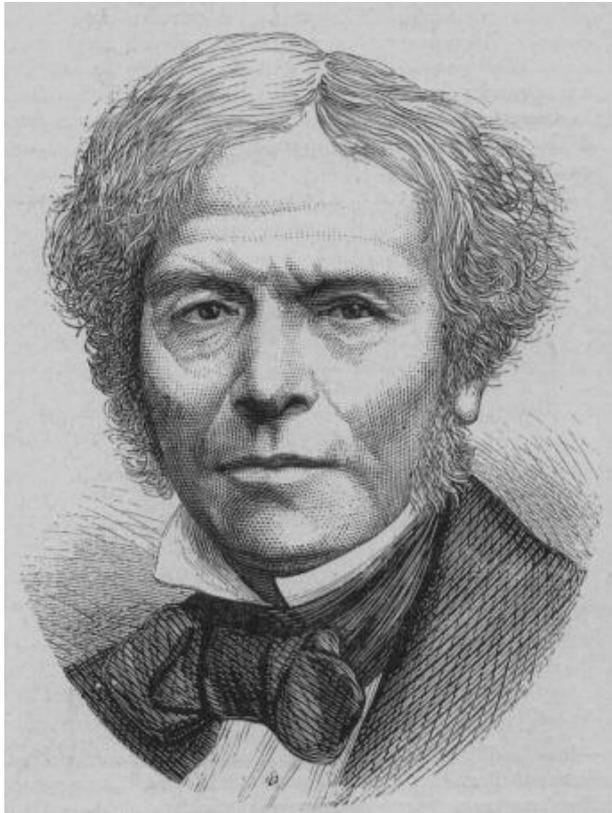
What is the story? What is the how and the why?

THE NARRATIVE

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'

WWW

THE INTERNET AND THE WEB

Scientific Data Value Chain

- Does the Web currently/have the potential to disrupt or support the data value chain?



The internet has also changed how we communicate with one another — and what is known as 'Web 2.0' is here. Blogs, social-networking sites, wikis and podcasts were alien concepts not all that long ago, but they are here to stay and some of them are significantly impacting the communication of science, and chemistry is no exception. Nature Publishing Group joined the chemical blogosphere back in March 2006 when we launched 'The Sceptical Chymist' blog and 'ChemPod' — a chemistry-themed podcast if you hadn't guessed. To reflect the firm inroads that chemistry seems to have made into the blogging culture, *Nature Chemistry* will feature a monthly column called 'Blogroll' that will round up stories that have caught the attention of the chemistry bloggers. Our first topics include a citation controversy and a reminder that boron isn't boring!

Nature Chemistry

Web 2.0 & Semantic Web

USER GENERATED CONTENT

QUALITY?

Accuracy



<http://www.opsrules.com/supply-chain-optimization-blog/bid/282916/Why-You-Shouldn-t-Waste-Effort-Improving-Forecast-Accuracy>

Beyond Open Access

05/12/2014

DIGITAL RESEARCH NOTEBOOKS

The Planning Process

Materials

Procedure

Into the Lab!

Into the Lab!

MoreTea: Tablet Interface and RDF World

Images and sketch commenting

LabTrove "preserving the record"

Transformation of plasmid JRH4712/66 into BW25141 by electroporation

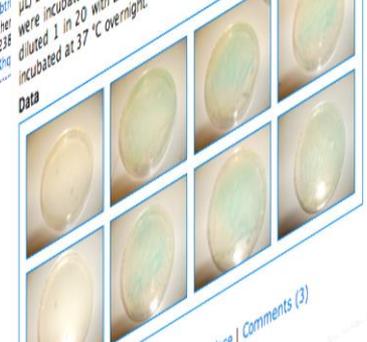
11th December 2006 @ 14:31

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

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

	-	+ve ctrl	-ve ctrl
BW25141	40 µL	40 µL	40 µL
plasmid 4712/66	0 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 appended. The transformants were diluted 1 in 20 with LB and 100 µL added to 100 µL amp arabinose plates and incubated at 37 °C overnight.



Jennifer Hale | Beta-glucuronidase | Comments (3)

- Archives
- January 2007 (24)
 - December 2006 (11)
 - November 2006 (5)
- Sections
- Beta-glucuronidase preparation and assays (18)
 - Beta-glucuronidase (18)
 - Data (Formatting) (1)
 - Software discussions (2)
 - Starting materials and reagents

- Lab Book Ref
- jrh4712-63 (1)
 - jrh4712-64 (2)
 - jrh4712-66 (1)
 - jrh4712-77 (1)
 - jrh4712-78 (1)
 - jrh4712-80 (1)
 - jrh4712-81 (1)
 - jrh4712-83 (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)
- Sample Parent
- jrh4712-74 (1)
 - jrh4712-76 (1)
 - jrh4712-76a (1)
 - jrh4712-77 (1)
 - 4712-78 (1)

05/12/2014

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

22nd January 2007 @ 11:37

Lab Book Ref: jrh4712-89

Sample Parent: jrh4712-80, blue

Sample Parent: jrh4712-80, white

Digestions were set up as follows:

	1	2	3	4	5	6	7	8	9	10	11
4712/80 blue	8 µL	-	-	8 µL	-	-	8 µL	-	-	-	-
4712/80 white	-	5 µL	-	-	5 µL	-	-	5 µL	-	-	-
p042	7.5 µL	7.5 µL	10.5 µL	10 µL	5 µL						
water	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL
EcoRI (a)	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL
EcoRI (b)	-	-	-	-	-	-	-	-	-	-	-
NcoI	-	-	-	-	-	-	-	-	-	-	-
EcoRI (a)	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL	2 µL
EcoRI (b)	0.5 µL	0.5 µL	0.5 µL	0.5 µL	0.5 µL	0.5 µL	0.5 µL	0.5 µL	0.5 µL	0.5 µL	0.5 µL
NEB buffer	-	-	-	-	-	-	-	-	-	-	-
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) assay date 2/05
EcoRI (b) assay date 7/05
Incubated in a waterbath at 37 °C for 3 hours.

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 - jrh4712-80 (1)
 - jrh4712-81 (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 Genemorph

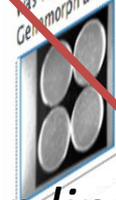
9th January 2007 @ 14:34

Lab Book Ref: jrh4712-78

Mutagenic PCR reactions were set up according to the following:

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

*GoTaq=1 µL stock + 3 µL water.
The reactions were run on program MUTAGB 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)

LabTrove: Easy Communication

Highly inter-linked report

Digital and Physical

Luke Marazzi's Y3 Chemistry Project

TLT660/4b Hot Stage Video

4th May 2010 @ 13:58



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Archives

- [April 2010 \(1\)](#)
- [March 2010 \(1\)](#)
- [March 2010 \(2\)](#)

Authors

Sections

- [Appendix \(1\)](#)
- [Samples \(3\)](#)

Tools

- [Show/Hide QR Code](#)
- [Show/Hide Keys](#)

QR Code



Sorlase Cloning - Mozilla Firefox

http://chemtools.chem.soton.ac.uk - barcode_print.php (application/p...

Done
start

05/

Southampton

Open Notebook Science

- Certainly not always the way to work!
 - IPR, Commercial, long term projects, recognition issues, etc

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

- But
 - Makes connection much easier if the data and processes are “Open”
 - Easy to export & access of “Linked-Data”





LabTrove Open Notebooks Mat Todd's Malaria Project

Praziquantel – Open Science

Head of an Invention Blog in Student Collaboration

Praziquantel Project

- Introduction
- Project Goals
- 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
- Separation of PZQamine

Powered by [LabTrove 2.2](#) © University of Southampton

Praziquantel – Open Science

Pictet-Spengler route to Praziquantel

Synthesis of intermediate and structure of PZQ

Synthesis of SC2-1

17th August 2012 @ 09:30

Sc 1-30

Synthesis of SC2-1 from tryptamine and 4-nitrobenzaldehyde

HRAC

Procedure followed

Pictet-Spengler route

Racemization of PZQ and PZQamine

Racemization of the enantiomeric 5-LiP-100-100amine obtained from racemic resolution of PZQamine

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

17th April 2012 @ 09:07

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

Archives

- April 2012 (6)
- March 2012 (6)
- January 2012 (4)

Sections

- Experiments (10)

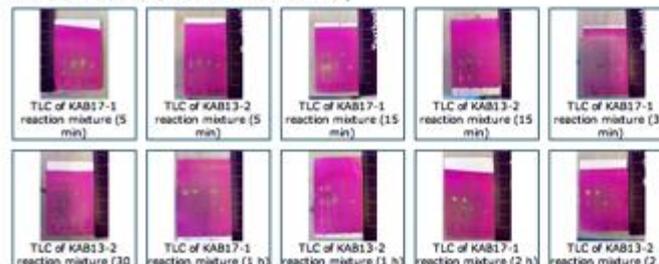
KAB17-1 (N-benzoyl PZQ analogue). Peptide Acetal KAB6-1: 373.1 mg (0.936 mmol), toluene: 37 mL, TFOH: 4.14 μ L (0.047 mmol, 5 mol%).

KAB13-2 (PZQ). Peptide Acetal KAB5-2: 394.2 mg (0.974 mmol), toluene: 39 mL, TFOH: 4.32 μ L (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 .



Racemic Resolution of Praziquantel and Praziquanamine

Separation of the enantiomers of Praziquantel and Praziquanamine by kinetic resolution

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

2nd August 2012 @ 09:30

Hazard and Risk Assessment:

Procedure

To a cooled solution of MNR7-6 (2.3 g, 85.13 mmol) in DCM (170 mL) at 0°C was added triethylamine (2.36 mL, 16.86 mmol) and benzoyl chloride (4.48 mL, 85.62 mmol). The solution was stirred for 14 hours at room temperature.

In the morning, the reaction was quenched with water (4mL) and stirred for 30 minutes after the

Sections

Racemic Resolution of Praziquantel and

Hydrolysis of PZQ

Hydrolysis of PZQ – WGPZQ101

17th June 2012 @ 09:30

Preliminary step in producing enantiomeric PZQ acid hydrolysis of

See also:

- Hydrolysis of PZQ – Standard Conditions (00-PZQ-1001)
- Hydrolysis of rac-PZQ (0002-110)
- Hydrolysis of rac-PZQ (0002-110)
- Optimizing the acid cleavage conditions 8

Procedure:

rac-PZQ (4.0 g, 12.8 mmol, MW: 312.1) was dissolved in a mL

Hydrolysis

LabTrove -> RSS -> Email / Twitter

My Recipes

Personal Shared Favorites

2 Personal Recipes, 2 turned on

Personal Recipes are a combination of a Trigger and an Action from your active Channels.

Filter -

if  **then** 

If new feed item from http://xray.orc.soton.ac.uk/feeds/xray_group/uid/2e575a007d7c25e2e54e672d1954b842?withcomments, then send me an email at

created less than a minute ago
never triggered

if  **then** 

RSS to Twitter

created February 25, 2014
last triggered April 02, 2014
triggered 10 times

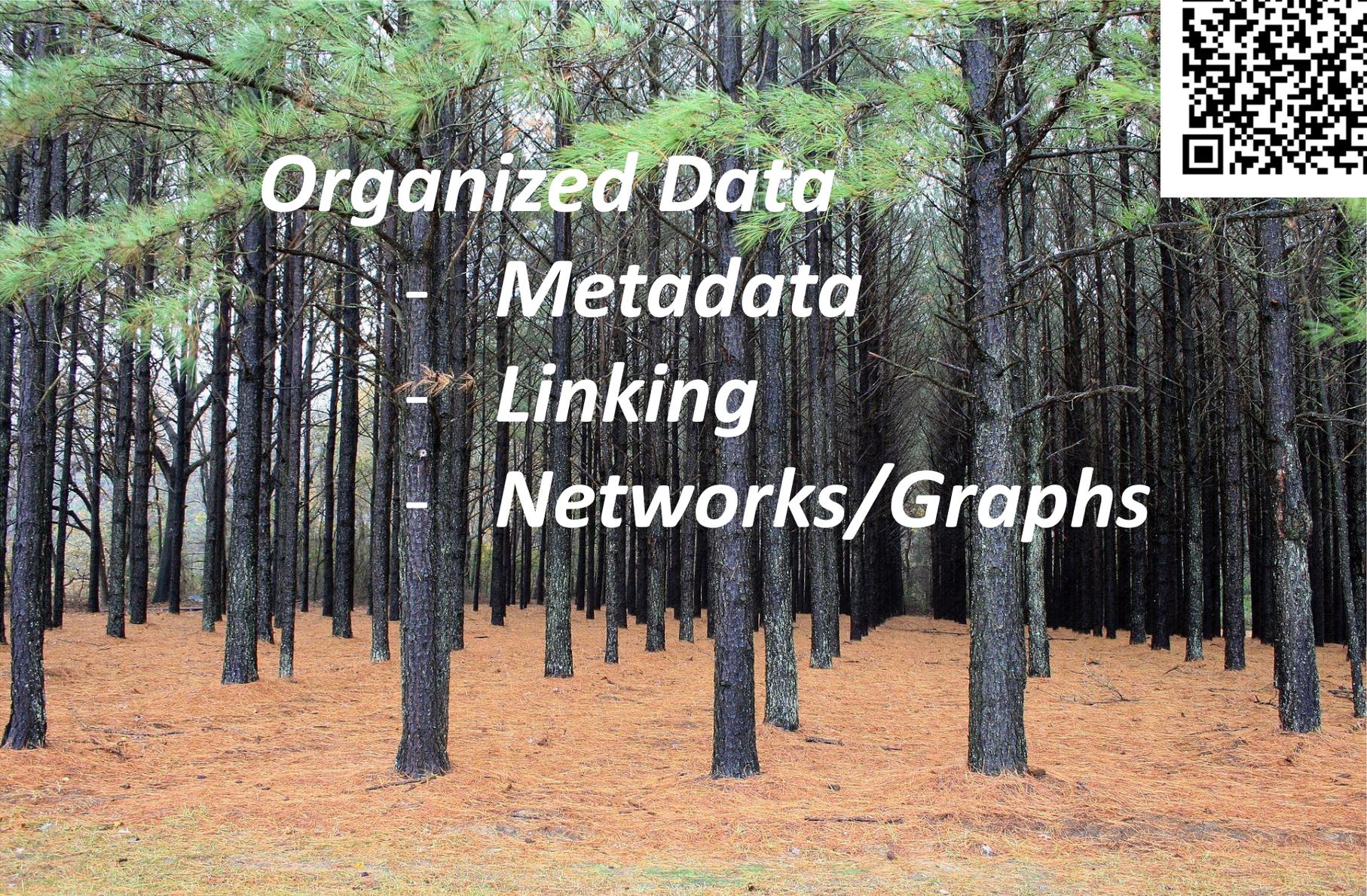


Finding the "Wood" From the "Trees"

http://upload.wikimedia.org/wikipedia/commons/4/41/Looking_through_the_Trees_in_Spearywell_Wood_-_geograph.org.uk_-_424274.jpg

05/12/2014

Beyond Open Access

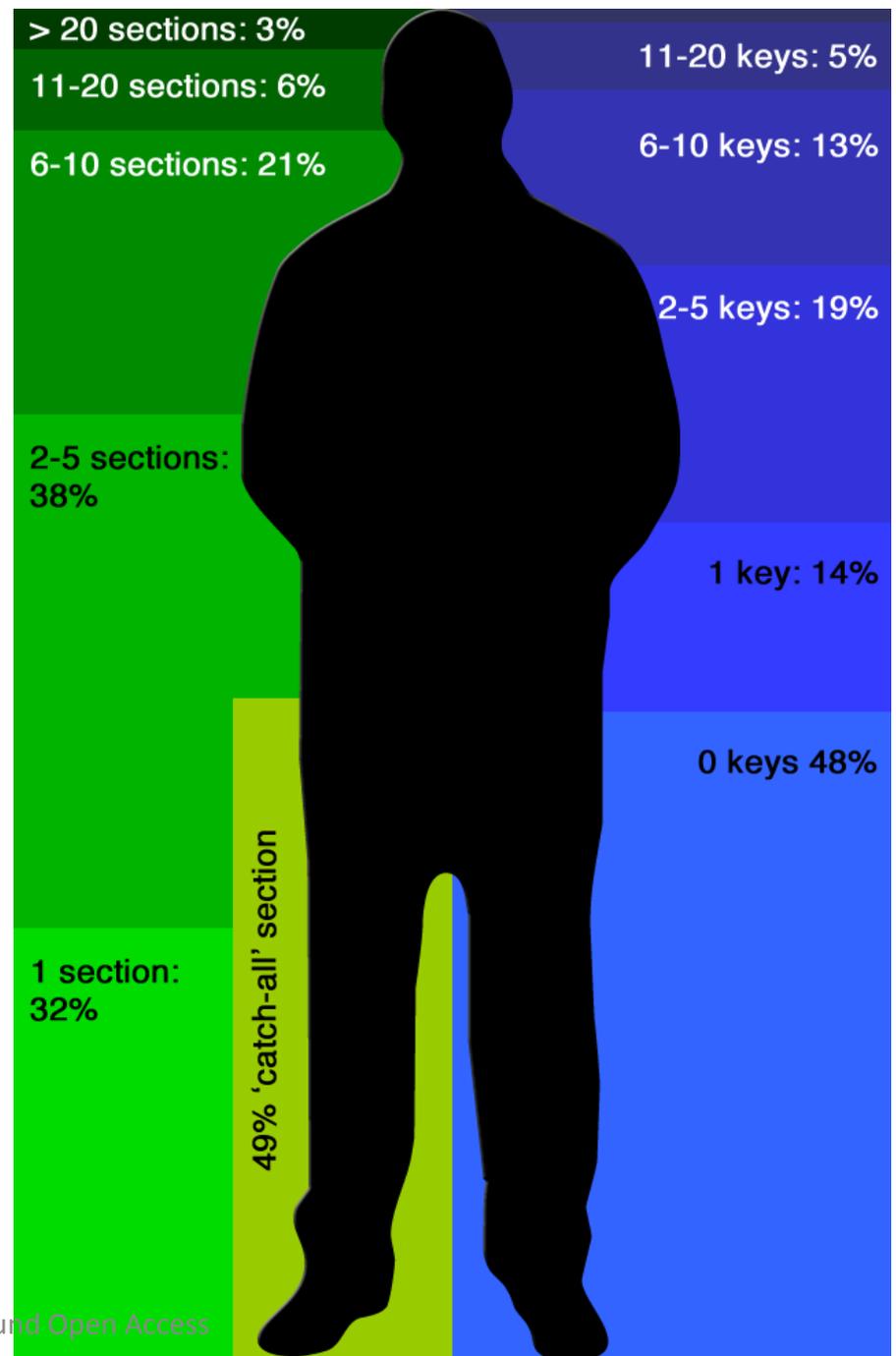
A photograph of a pine plantation with many tall, thin trees and a ground covered in brown pine needles. The text is overlaid on this image.

Organized Data

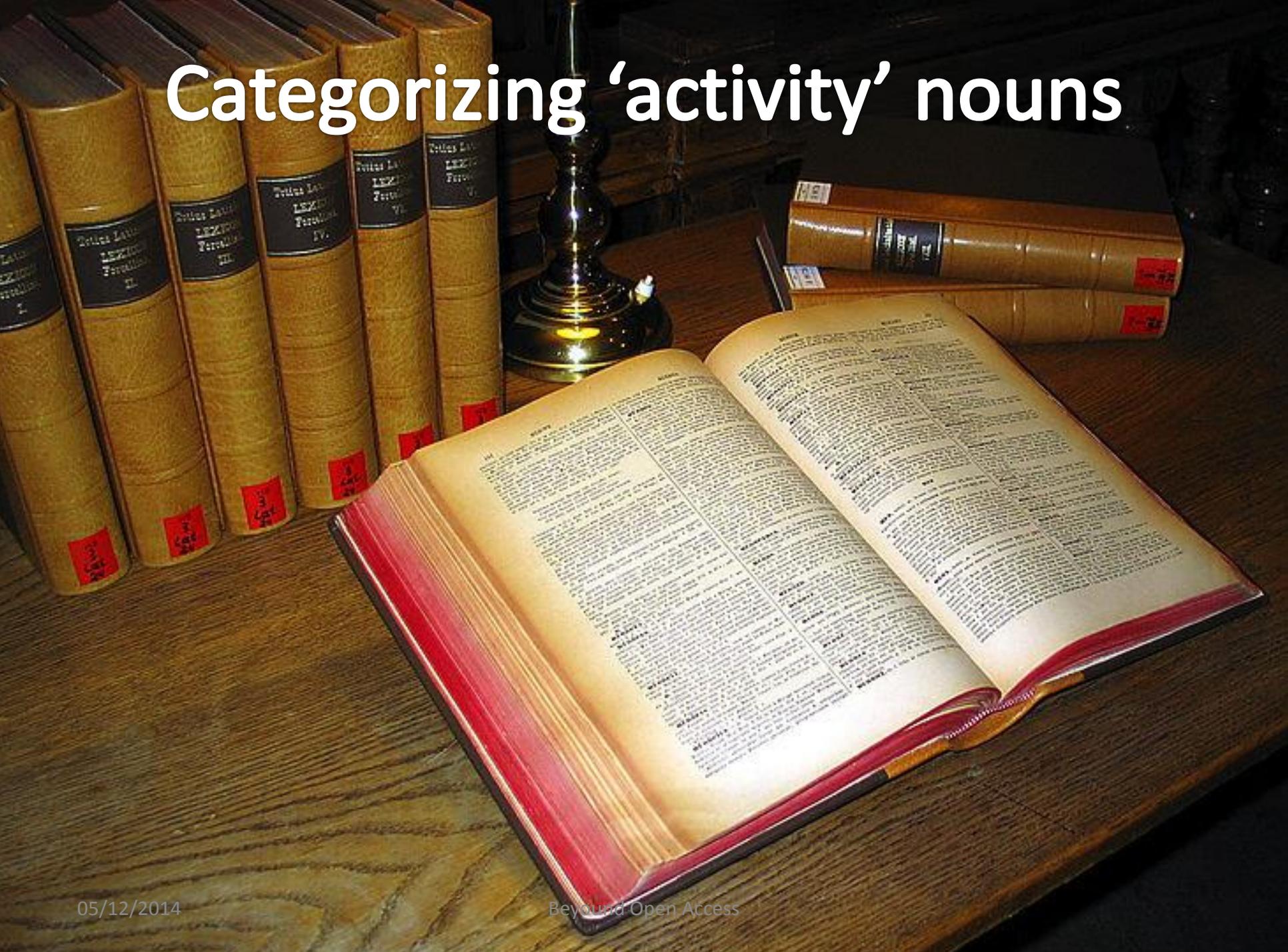
- *Metadata*
- *Linking*
- *Networks/Graphs*

http://en.wikipedia.org/wiki/Plantation#mediaviewer/File:Pinus_taeda_plantation.jpg

A big proportion of our users are not really adding metadata!



Categorizing 'activity' nouns



NASA results



Metadata

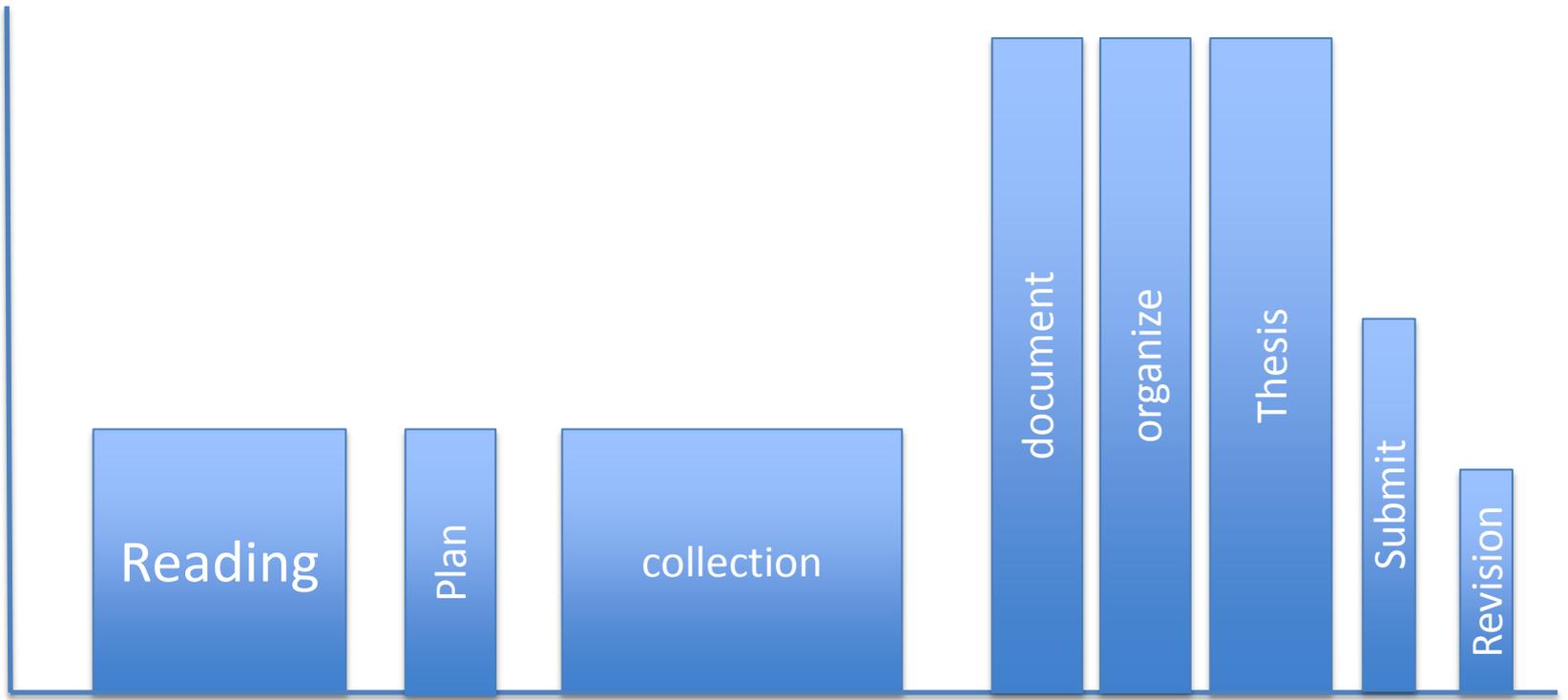
- User Created
- Metadata Sentence
 - Attempt to get verbs (processes) as well as nouns (things)

Toki Pona



http://en.wikipedia.org/wiki/Toki_Pona

Effort



Time



Research student thesis writing often involves dealing with the consequences of having delayed the (huge) organization effort to the point of writing up

Smart Tea Project



the Smart Tea Project

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

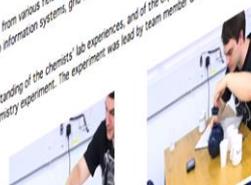
- Chris,
a real chemist, on using Smart Tea
instead of a paper lab book.

chemists doing chemistry - within an
analysis and dissemination of

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 in particular, we made tea as a chemistry experiment. The experiment was lead by team member Graham Smith, a chemist and



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, processed within the global science community.

Project is focusing on the experimental process itself in order to capture and written information generated in the lab and processed through the confines of a single

P2 - Plans & Provenance

Backs

When chemists run experiments, they record those hypotheses, they reference those hypotheses, the modern lab experiment recorded using the same tools as scientists have been using over the 200 years: a bound paper lab book (pictured right).

The flexibility of the lab book makes it great for chemists while carrying out an experiment: they can move it easily from their desk to the lab bench to a shelf. The book itself, however, is a poor mechanism for making the information stored in that book available to other scientists within the lab, or for that matter: to the same scientist after the experiment has been completed: if the scientist does not have the lab book to hand, the information is unavailable.



The Lab Aether

With the evolution of the Semantic Grid and Pervasive Computing (think 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 medium holding information being generated within the lab. As chemists build up an experiment, they rely on that information being 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.

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"

[British Standards Institute](#),

enter standard no.:
BS6008:1980 (6 pages,
£22.00)

[Guardian story](#) (and [abbreviated version](#)) of this BSI [prize winning](#) document.

[Counterfeit tea](#) (or [smouch](#))

- The BBC (and Michael Quinion for the explanation of smouch)

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

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 S

C₁₄H₂₀O₅

InChI=1/C14H20O5

Identificati
Numb

Control
Keyword

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

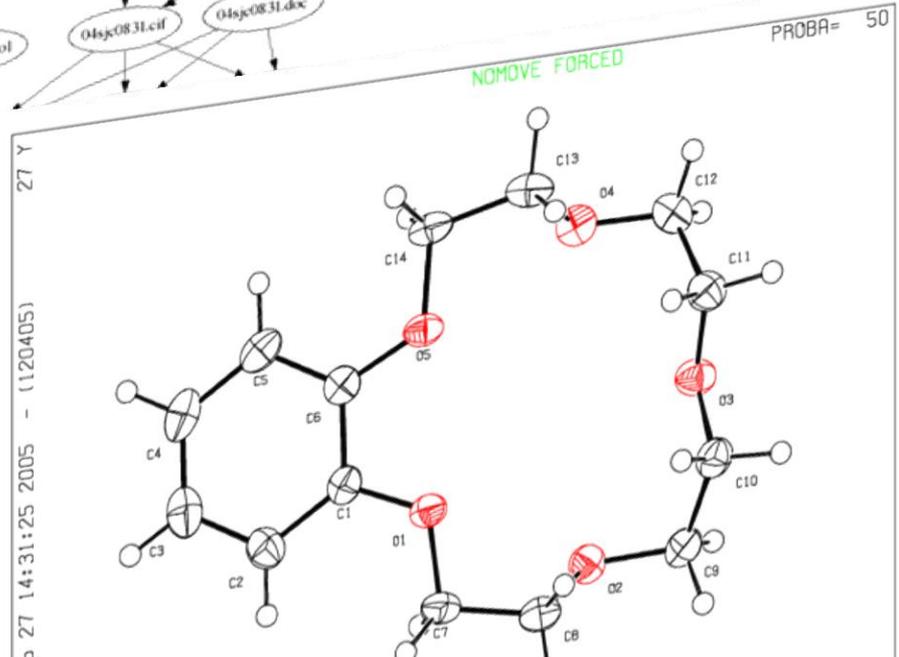
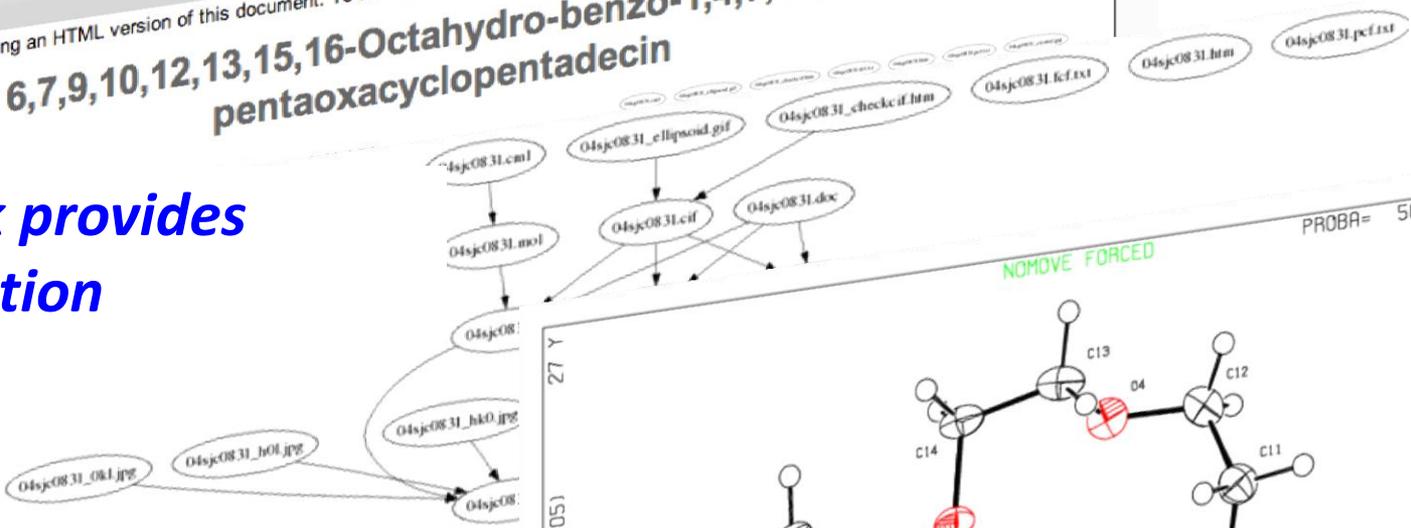
Graph/Network provides intuitive navigation

Depositor
Structure alr
project.
Data colle
Chemical fo

Creator: CUN
Creator: Hun
Date: 200

Stages (10)

Stage:	Pl:
1	plan.rdf
2	plan.rdf



VALIDATION

Publication@Source

“The Laboratory”

- A laboratory is an Integration of people and equipment
- A complex socio-technical system
- Disrupted or integrated by digital infrastructure?
- How to support (a) people to do what they are best at doing and (b) computers to undertake what they can do best and (c) ensure that they can work together.



Bringing dissemination in to the lab... use and re-use of data... the digital research notebook

DISSEMINATION IS PART OF THE RESEARCH

“Engrooved*”

* concept highlighted in teaching by Paul Trowler

- <http://www.brad.ac.uk/sustainable-universities/media/sustainableuniversities/Keynote-Prof-Paul-Trowler.pdf>



<http://www.todayandtomorrow.net/2010/02/22/quarter-mile-groove/>

The System

adapted from Atul Gawande 2014 Reith Lectures

- “Primitive idea”
 - You ought to do x.
- Medieval approach
 - You **must** do x! You must follow the standards
 - Will will take away your grant....!
- Modern world(?)
 - Becomes the norm, make it easy to do
 - Checklists
 - ***Feedback loops***

We must speed up the knowledge discovery process



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From *The New Yorker Book of Technology Cartoons*.

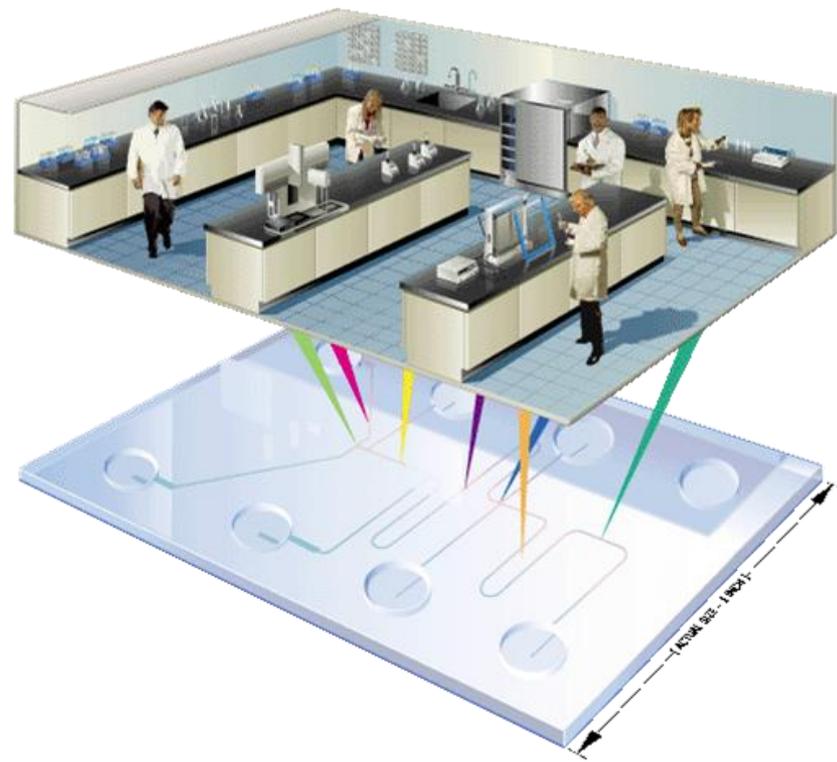
*All I am saying is that now is the time to
develop the technology to deflect an asteroid*



Re-imagining Scientific Research

A “Social Machine” of experienced
researchers, technology &
information

<http://lab-on-chip.gene-quantification.info/>



LABORATORIES OF THE FUTURE

The Lego Movie

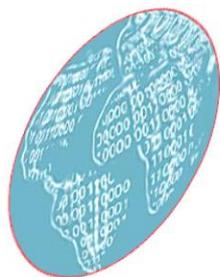


*Everything is Awesome,
Everything is cool when you're part of a team*



IDCC 2014 Meeting San Francisco

<http://www.dcc.ac.uk/events/idcc14/programme-presentations>



**Got Data?
Building a Global Ecosystem
for Data-Driven Innovation**

Dr. Francine Berman

Chair, Research Data Alliance / US
Edward P. Hamilton Distinguished Professor in
Computer Science, RPI

**Lucile Packard
Children's Hospital
AT STANFORD**



**Big Data in Biomedicine:
Discovering new drugs and diagnostics
from a trillion points of data**

abutte@stanford.edu
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Atul Butte, MD, PhD
Chief, Division of Systems Medicine,
Department of Pediatrics, Genetics,
and by courtesy, Medicine, Pathology, and
Computer Science
Center for Pediatric Bioinformatics, LPCH
Stanford University



Fran

NCBI Resources How To

GEO DataSets **breast cancer** Search

Display Settings: Summary, 20 per page, Sorted by Default order

Filters: Manage Filters

Top Organisms [Tree]

- Homo sapiens (38361)
- Mus musculus (3059)

Results: 1 to 20 of 41593

dbGaP GENOTYPE and PHENOTYPE

Entry type

- DataSets (141)
- Series (1582)**
- Samples (39835)**
- Platforms (35)

Organism

Select ...

Study type

Expression profiling by array

Methylation profiling by array

More ...

Author

Select ...

Attribute name

tissue

strain

More ...

Publication

Public bio

1. Leukemia

2. Co-expression of HER3 in three-dimensional cell cultures

Embargo Release

Feb 13, 2009

Details

Participants

1931

14277

2875

Type of Study

Case-control

Longitudinal

Case-control

Parent-offspring

Study

By Studies

By Diseases

Advanced Search

CIQR: Genome-Wide Association Study in Familial Parkinson Disease (PD)

Framingham SHARE

GAIN: Collaborative Association Study of Glioblastoma (GAIN) by Proton

GAIN: Genotyping the 270 HapMap samples for GAIN by Proton

GAIN: Genotyping the 270 HapMap samples for GAIN by Proton

GAIN: International Multi-Center ADHD Genetics Project

GAIN: Linkage Genome-wide Association Study of Schizophrenia

GAIN: Major Depression: Stage 1 Genome-wide Association Study

GAIN: Search for Susceptibility Genes for Diabetic Neuropathy

GAIN: Whole Genome Association Study of Bipolar Disorder

GWAS: Framingham and Simulated Data

Genome-wide Association Studies in the Hutterites

Genome-wide Association Study of Neuroblastoma

Genome-wide Study in Amyotrophic Lateral Sclerosis and

Genome-wide Study in Amyotrophic Lateral Sclerosis and

Ischemic Stroke Genetics Study (ISOGS)

Macro-Paragon LEAPS (United Efforts to Accelerate Parkinson's Disease-Related Eye Disease Study (AREDS))

NINDS Parkinson's Disease

NINDS Parkinson's Study

NINDS Repository Cerebrovascular Disease/Stroke Study

NINDS Repository Motor Neuron Disease/ALS Study

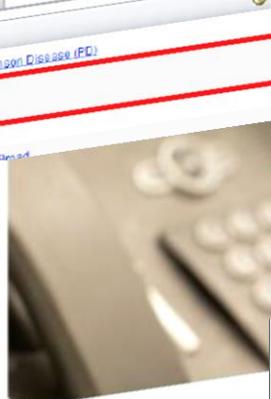
NINDS Repository Neurologically Normal Control Cohort

POPRES: Population Reference Sample

SEARCH: GWAS Study of Strain-Induced Myopathy

Study of Irish Amyotrophic Lateral Sclerosis (SALS)

The Finland-United States Investigation of NIDDM Genetics



conversant bio products services company

search keyword or disease

your cart is currently empty contact us: (866) 333-3333

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Home > Peripheral Blood | Plasma | Leukemia

Peripheral Blood | Plasma | Leukemia

SKU: PBL-PLA-LE

\$55.00

Quick view: 1.0ml Plasma specimen collected in K2EDTA tube and stored in 1.0ml cryovial. Sample stored at -80C and shipped on dry ice.

Disease subtype

-- Please Select --

Units

-- Please Select --

add to cart

add to saved items Email & C

Overview > Product Reviews >

Additional Information

SKU

Treatment Status

PBL-PLA-LE

Any Treatment, Pre Treatment, Post Treatment, Active Treatment, Recurrent/Refractory Disease, Remission

The samples you need may already be available

THE AUTOMATED LAB

Start-up firms say robotics and software that autonomously record every detail of an experiment can transform the efficiency and reliability of research.



http://www.nature.com/polopoly_fs/1.16429!/menu/main/topColumns/topLeftColumn/pdf/516131a.pdf

The Art of Asking the Right Question

Are You Asking The Right Question?

+ Comment Now + Follow Comments

Forty years ago, someone asked a profound question that fundamentally changed how we communicate with each other every day. At the time, I was nine years old living in South Africa. When our family visited my grandfather's farm for the holidays, the telephone we used was a "party line", where we would listen for the pattern of rings when the telephone rang to determine if the call was for us or for the next farm over. Hard to believe now—it does not seem that long ago.

At the same time, Marty, a young engineer at Motorola, was given a new assignment. He was asked to lead a team on a project that showed great promise—the next generation of a car radiotelephone. Marty accepted the challenge. However, instead of jumping in, he stepped back and paused, which led him to ask himself a very insightful question.

"Why is it that when we want to call and talk to a person, we have to call a place?" That nagging, insightful question changed the entire trajectory of his work, as he refocused his team's attention on untethering a person from a place (including a car).



Want to Lead? Learn to Ask the Right Questions

by **BIG THINK EDITORS** MAY 22, 2014, 12:00 AM



Have you ever walked away from a sales meeting wondering what you could have said differently to a potential client? Or do you feel as though you're only wasting your breath trying to convince your employees to believe in a new initiative or direction? Are you tired of telling your children to clean up their rooms? Convincing others can't come from you—it has to come from them. How does this happen? Learn to ask the right questions.

Daniel Pink is a management expert and the author of five bestselling business books, including *Drive*. He stopped by *Big Think*'s studio to talk about his latest book *To Sell is Human: The Surprising Truth About Moving Others*.

*He who asks a question is a fool for five minutes;
he who does not ask a question remains a fool forever.*

—Chinese Proverb

Quora Search for questions, people, and topics

SHARE QUESTION

Like 0 Tweet 0

RELATED TOPICS

- Macroeconomics
- Monetary System
- Currencies
- Virtual Currency
- Credits (Quora feature)

Why is asking a good question on Quora (20 credits per follower) more rewarding than writing a good answer (10 credits per upvote)?

Follow Question 24

5 ANSWERS ASK TO ANSWER

Quora User, Quora Admin
42 upvotes by Vikas Prajapati, Quora User, Quora User, (more)

The reasons are quite straightforward:

The average return from:

- A question = $20 \times$ Number of followers
- An answer = 50 for OP's upvote + $10 \times$ Number of upvotes

Now (and this is a *post hoc* assumption) the average number of upvotes per answer is more than the average number of followers per question, so it makes sense to incentivize question addition by giving more weightage to number of followers.

You should also remember that questions drive Quora; without interesting questions there'd be no interesting answers.

Updated 30 Dec, 2013.

Upvote 42 Downvote Comments 2+

Related Questions

- Will Quora's credits result in more mundane questions being answered?
- How many credits do you get for upvotes on answers? And does the author of the question get any credits?
- What is the goal of Quora Credits?

Why is asking a good question on Quora (20 credits per follower) more rewarding than writing a good answer (10 credits per upvote)?

<http://www.quora.com/Why-is-asking-a-good-question-on-Quora-20-credits-per-follower-more-rewarding-than-writing-a-good-answer-10-credits-per-upvote>

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- My research group
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- My colleagues
 - Chemistry, Physics & ORC, Computing, Engineering,
 - Statistics/ Mathematics
- Funding
 - University of Southampton, Chemistry
 - EPSRC, RCUK, JISC/Jisc, IBM, Microsoft, TSB, Lonza

Thank you for listening



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from *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