

Science Ajar

The future of research: are you ready?

Jeremy G. Frey
15 March 2013



ProfeChem

Jisc Digifest

Light Microscope

UltraFast Xray Group

[<< Next Post](#)

[Previous Post >>](#)

Search

Timeline

- 1-SWAMP
- 2 micron diffraction pattern
- SiN AI
- Microscope images
- Change to Matlab licensing on Iridis
- Hello!
- Zr and Nb data
- Grid diffraction through focus
- 2 micron fib sample maps
- Micro and Nano sensors workshop
- Hippocampal sample progress
- GPU coding initial work for SYMBIOSIS
- XUV spectrometry update
- Grid diffraction data from monday

tracts from next months NLO conference

11/03/2014

Jisc Digifest

Aug

CabinetOffice

About the Cabinet Office | National Security | Constitutional Reform | Government Efficiency | Transparency | Big Society | Government that works

Open Data White Paper and Departmental Open Data Strategies

28 June 2012

Open access workshop

The Royal Society
Monday, February 25th, 2013 10:00 AM - 12:00 PM
London, United Kingdom

Open Data White Paper: Unleashing the Potential

Expanding access

Report of the Working - the Finch Group

Science as an open enterprise

Final report

21 June 2012

Intelligent Open Access to Data

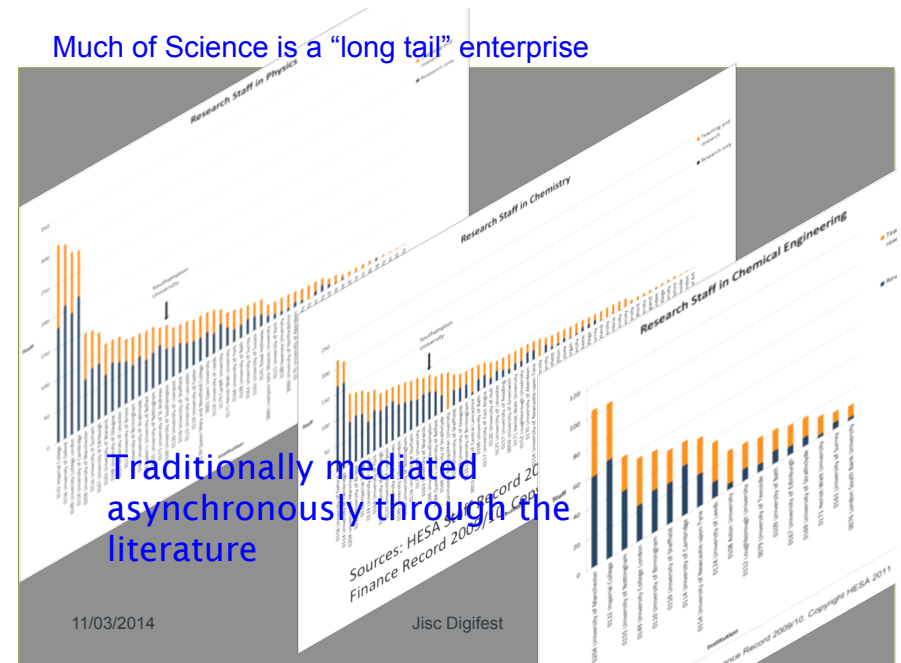
11/03/2014

Intelligent Open Access to Data

11/03/2014

Jisc Digifest

Much of Science is a “long tail” enterprise



Traditionally mediated
asynchronously through the
literature

Sources: Finance Record 2

Jisc Digifest

2008 Record 2009/10 Copyright HESA 2011



11/03/2014

Jisc Digifest

© Cartoonbank.com



What is the story? What is the why?

THE NARRATIVE

11/03/2014

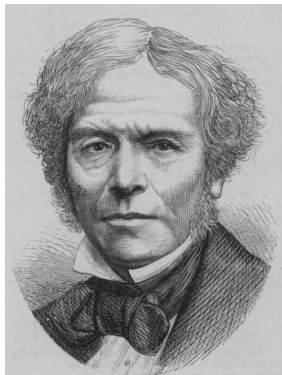
Jisc Digifest

6

ON BEING A SCIENTIST

A GUIDE TO RESPONSIBLE CONDUCT IN RESEARCH
THIRD EDITION

Scientific Narratives



11/03/2014

Jisc Digifest

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'

RESOURCING

11/03/2014

Jisc Digifest



- Co-sourcing
- In-Sourcing
- Out-sourcing
- Net-Sourcing
- Open Sourcing
- Single-Sourcing
- Crowd Sourcing

11/03/2014

Jisc Digifest

breast cancer

Peripheral Blood

Publicly available

The samples you need may already be available

11/03/2014

Jisc Digifest

IDCC 2014 Meeting San Francisco

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

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

Atul Butte, MD, PhD
Chief, Division of Systems Medicine, Department of Pediatrics, Genetics, and by courtesy, Medicine, Pathology, and Computer Science
Stanford University

Butte Lab

11/03/2014

Jisc Digifest

Some projects need large amounts of data from the literature: access can be an issue

Digital Repository

E-BANK

PERPETRATOR OF A DARING DAYLIGHT ILLEGAL ELECTRONIC TRANSFER OF FUNDS FLEEING THE SCENE OF THE CRIME

Data

11/03/2014

Jisc Digifest

Scroll down to browse a list of available research models for **Type I and Type II diabetes, hyperglycemia, insulin resistance, diet-induced obesity and related diseases**. Use the filters on the left to refine the list and then click on any listing to view technical information or to ask a question.

Click on the Vendors tab to view a complete list of CROs that offer diabetes and obesity pharmacology models.

Search Filters

Diabetes and Obesity

BB/W Rats
Feed Intake
Goto-Kakizaki Rats
Non Obese Diabetic Mice
Obese Mice
Obese Primates
Primate Diabetes
Streptozotocin Mice
Streptozotocin Rats
db/db Diabetic Mice
fa/fa Zucker Diabetic Rats

Certifications

GLP (48)
AAALAC (28)
GMP (20)
ISO 9001 (7)
GCP (7)
FDA (5)
USDA (4)

11/03/2014

VIEW SERVICES **VIEW VENDORS** 133 results [get help](#)

Univ. of Maryland School of Medicine Obesity and Diabetes Research Center
University of Maryland School of Medicine Obesity and Diabetes Research Center focuses on research in obesity, diabetes, and aging in nonhuman primates.

Transgenic Rabbit Models
Transgenic rabbits are transgenic rabbit models for the study of atherosclerosis, ophthalmology, hypertrophic myopathies, diabetes, obesity, hemostasis, respiratory diseases, AIDS, and cancer.

Ophthalmic Services
Ophthalmic model services for macular degeneration, diabetes, uveitis, and dry eye.

PharmaNess
PharmaNess offers pharmacokinetics, pharmacodynamics, formulations, behavioral assay, in vivo screening, ex vivo screening, microscopy, stereology and histology staining services.

Wisconsin National Primate Research Center
Wisconsin National Primate Research Center focuses on research of regenerative medicine, reproduction, immunology, virology, aging, and metabolic diseases.

Are you a vendor?
Visit our Backoffice to find out how you can offer your services on Assay Depot.
[Visit the Backoffice >>](#)

Request a demo
Contact Corey Jacklin to schedule a demonstration
215-369-0965
jacklin@assaydepot.com

Ask An Expert
Use our free service locator program to find the research services you need.

Search PubMed
Search PubMed for "Diabetes and Obesity" using BioWizard.

Selected Vendors

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

DISSEMINATION IS PART OF THE RESEARCH

11/03/2014

Jisc Digifest

Smart Tea Project

the Smart Tea Project
"I can go anywhere and use this, this is me and my data. Its all there, long."

Smart Tea
The Smart Tea Project is a research project that aims to create a smart tea bag that can be used to collect and analyze data from a variety of sources, including the internet, social media, and other data sources.

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

P2 - Plans & Provenance

11/03/2014

Jisc Digifest

The Planning Process

Materials

Procedure

Into the Lab!

Into the Lab!

MoreTea: Tablet Interface and RDF World

11/03/2014

LabTrove preserving the record

Images and sketch commenting

Transformation of plasmid JRH4712/66 into BW25141 by electroporation

11/03/2014

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

Mutagenesis of plasmid p042 via Taq and Genomorphi

LabTrove: Easy Communication

Highly inter-linked report

Set up your own publishing operation!

Publishing Open Research Data

ju[ubiquity press
open scholarship

Brian Hole, Founder and CEO
IDCC Research Data Publication in Principle and Practice workshop, San Francisco
February 24 2014

11/03/2014 brian.hole@ubiquitypress.com www.ubiquitypress.com / @ubiquitypress

Digital and Physical

Luke Marazzi's Y3 Chemistry Project

TLT660/4b Hot Stage Video

4th May 2010 @ 13:58

View Source | Samples | Comments (0)

Add comment to Post

Text*

Re: TLT660/4b Hot Stage Video

QR Code

Impact on researchers

Comparison with traditional paper notebooks

Electronic Laboratory Notebooks
ELNs

Communication
Collaboration
Sharing
Linking
Curating

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

11/03/2014 Jisc Digifest

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”

11/03/2014

Jisc Digifest

Search: ElabTrove

Public Blog Post: Synthesis of 1-amino-2-methyl-1-oxopropan-2-yl 1-(4-fluorophenyl)-2,5-dimethyl-1H-imidazole-5-carboxylate... <http://t.co/0vD17> #malaria #drugdesign

Public Blog Post: 1H-NMR Experiment to determine the water content of thieno[3,2-d]pyrimidin-6-yl benzenesulfonamide... <http://t.co/GnTcN09l> #malaria #drugdesign

labtrove, [H] Fri 17 Aug 05:33 via twitterfeed

RT @TVLMed: Daily #TravelHealth Tips (#TVLMed) is out! <http://t.co/UJNtoGQSV> Top stories today via @BiblioBuster @labtrove @a100ciacerta

Ronan Kelly 13, [H] Thu 16 Aug 11:27 via PaperJi

Public Blog Post: Synthesis of 3-(4-ethoxyphenyl)-2,5-dimethyl-1H-imidazole-5-carboxylate... <http://t.co/yPelaSUx> #malaria #drugdesign

labtrove, [H] Thu 16 Aug 07:19 via twitterfeed

labtrove, [H] Thu 16 Aug 07:19 via twitterfeed

Public Blog Post: Synthesis of 3-(4-ethoxyphenyl)-2,5-dimethyl-1H-imidazole-5-carboxylate... <http://t.co/UJNtoGQSV> Top stories today via @BiblioBuster @labtrove @a100ciacerta

LabTrove Open Notebooks Mat Todd's PZQ Project

PZQ

Praziquantel - Open Science

Pictet-Spengler route to PZQ

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

KAB17-2 (PZQ). Peptide Acetal KAB-2: 394.2 mg (0.974 mmol), toluene: 39 mL, TIOH: 4.32 µL (0.048 mmol), 5 mol%.

Racemic Resolution of Praziquantel

Monitoring the Reaction Progress by TLC

Hydrolysis of PZQ

Introduction

11/03/2014

Jisc Digifest

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



Publication@Source

11/03/2014

Jisc Digifest

Blog Syn

Crowdsourcing meets Organic Synthesis. Speed and Aplomb.

Blog Archive

▼ 2013 (5)

► March (1)

▼ February (2)

Blog Syn

#003:

Benzylic

Oxidation of

Arylmethane

& ...

Blog Syn

#002:

Pd-Catalyzed

4-Cy

Selective

C-H Olef...

► January (2)

Tuesday, February 12, 2013

Blog Syn #003: Pyridines

(Disclaimer: The following observations gleaned stay close to the original, cropped and scaled to fit)

Updated: 2/20/13 - Add

Ref: Yu, M.; Gao, G.-L.;

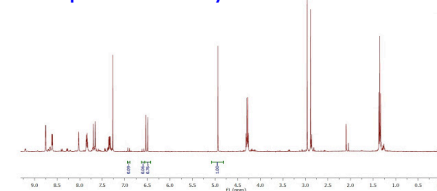
Experimenters: Two - Si

Recommendation: Pendi Initial - Moderately repro with literature. May requi

General scheme:



This is a picture - why has the data been lost?



The ratio I get from these integrations is 12.7 / 1.5 / 1.1 (m/o/p), which agrees with the original publication.

Update (2/20/13): Prof. Yu indicates that integration of the crude against 0.5 equiv. of CH₂Br₂ (4.94 ppm, above) gives an NMR yield of meta-olefination product matching the literature (76%).

Of note, the reagents are quite different - he's using a higher grade of both (1,10-phen) and pyridine, but we don't have information on the acrylate used or the Pd source. Also of note, the 50 mL long, cylindrical tube volume clearly benefits the reaction, as alluded to in Prof. Yu's original email.

We thank Prof. Yu for sending along some clarification. Perhaps this signifies a change in the way reactions are reported; if everyone had to send along photo evidence, would there be so many reproducibility issues in the modern literature?

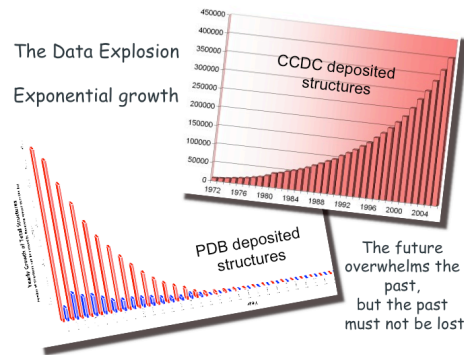
Jisc Digifest

-SAO

11/03/2014

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?



11/03/2014

Jisc Digifest

BACK TO PLANS & PLANNING

11/03/2014

Jisc Digifest



"In theory, there is no difference between theory and practice. But, in practice, there is."

Unknown (possibly Yogi Berra or Manfred Eigen)

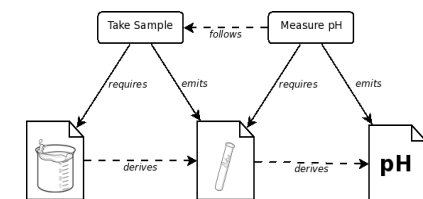
11/03/2014

Jisc Digifest

27

P&E Ontology: Planning

- Prospective provenance
- Describes a scientific experiment that *will be enacted* (in the future)
- Three entity types:
 - Plan
 - Plan Stage
 - Plan Object

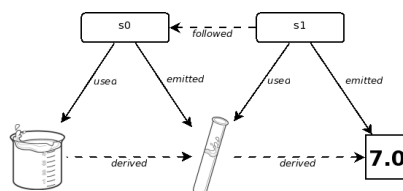


11/03/2014

Jisc Digifest

P&E Core Ontology: Enactment

- Retrospective provenance
- Describes a scientific experiment that *was enacted*
- Three entity types:
 - Run
 - Stage
 - Object



11/03/2014

Jisc Digifest

29

Change in the whole way we design and build

WHAT CAN WE LEARN FROM LEGO

11/03/2014

Jisc Digifest

3D Printers: A radical change to the experimental section of a paper!

Thanks & Acknowledgements

- UK e-Science & Digital Economy Programmes
- RCUK: EPSRC, BBSRC & TSB, JISC/HEFCE, Microsoft & IBM, for funding and support
- Southampton Colleagues and Students from Chemistry, Electronics & Computer Science, Engineering, Mathematics/Statistics, iSolutions and the Library
- Colleagues at Bath/UKOLN, Oxford/OeRC, STFC, Reading, Penn State, Cornell, PNNL, UNSW, USyd

11/03/2014

Jisc Digifest



Thank you for listening



"Trust me Mort
vast i

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

11/03/2014

Jisc Digifest