



Digital Chemistry

Reducing and Managing Uncertainty
Chemistry 2.0 (or 3.0)

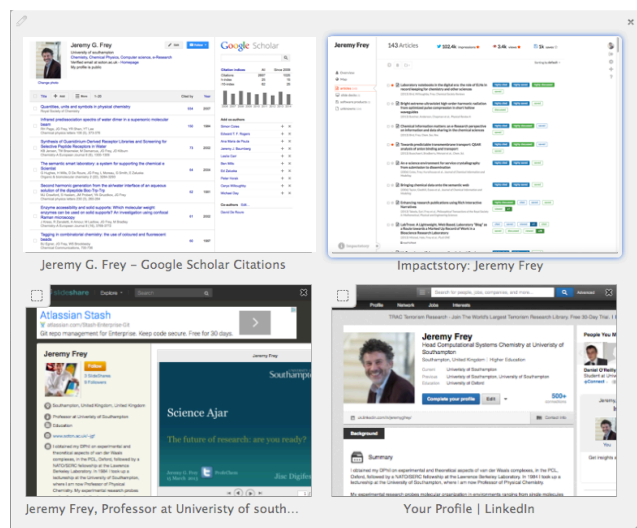


© Cartoonbank.com

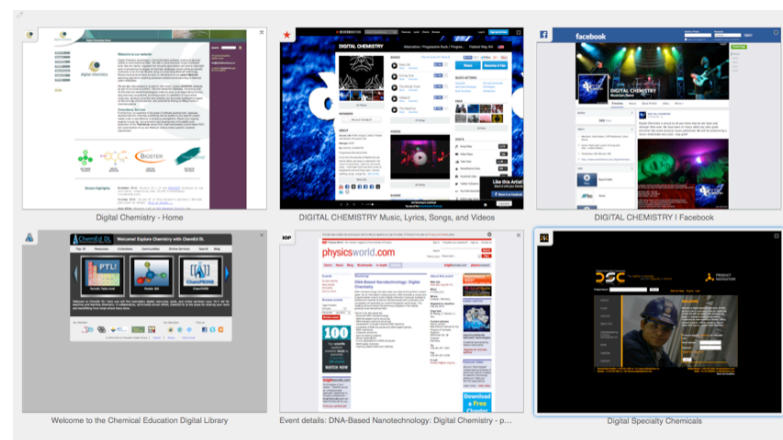


"We have lots of information technology. We just don't have any information."

A Chemist's Digital Aura



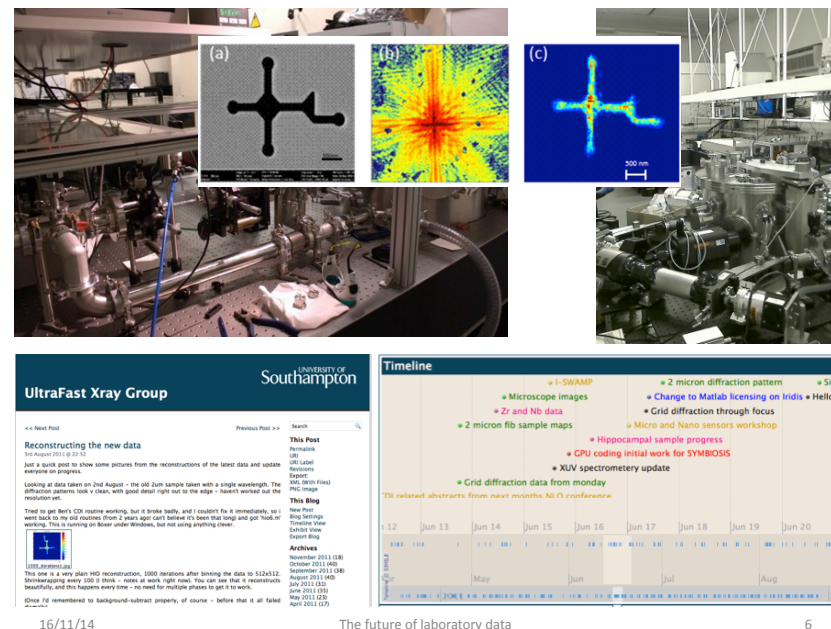
Google "Digital Chemistry"



But also note that my search results will probably not be the same as yours!

Outline

- Introduction
- Computational Chemistry and Computational Support for Chemistry Researchers
- Open Access vs Intelligent Access to Data
- Digital Notebooks & Data Citation
- The Future

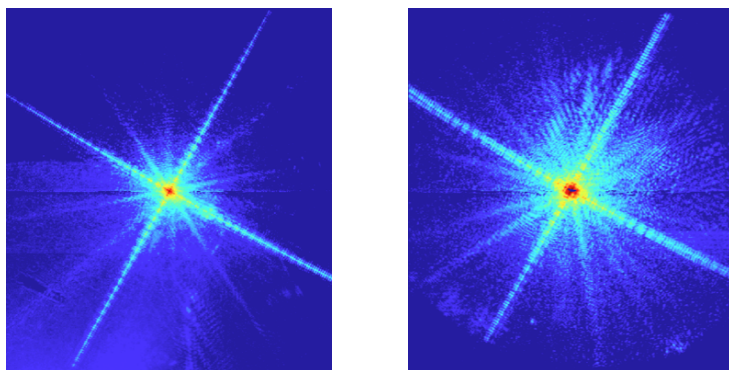


16/11/14

The future of laboratory data

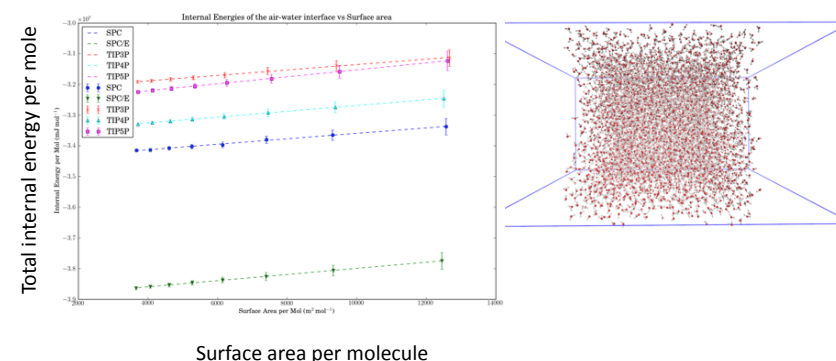
6

Coherent diffraction Imaging for lens-less 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.

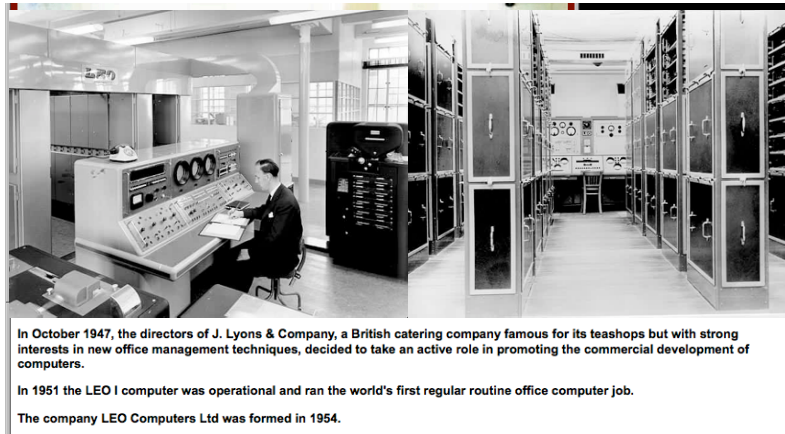
Air/Water slab MD simulation



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.

Lyons Electronic Office (LEO) 1951

Information Transformation

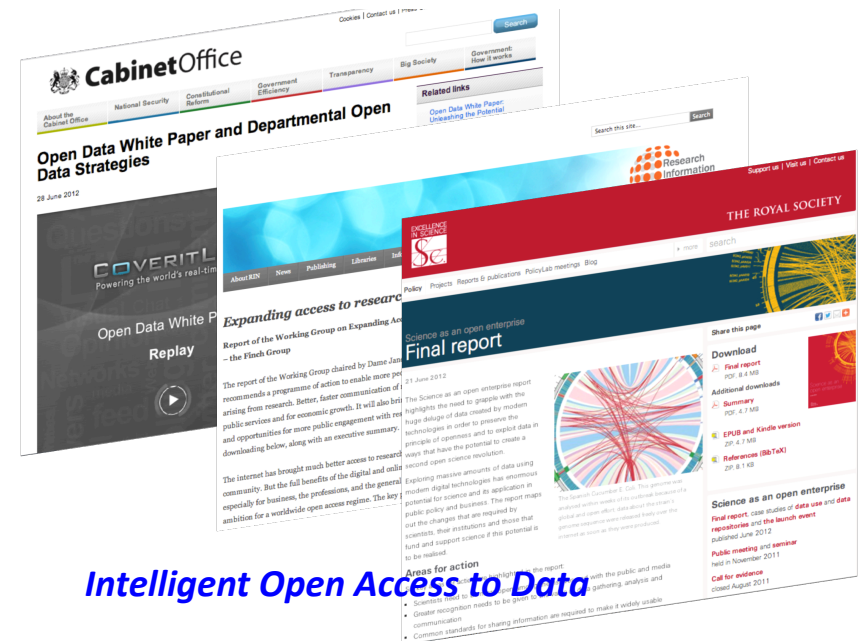
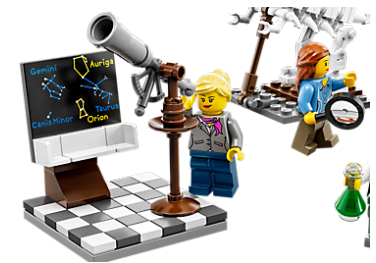


Collaboration

- Research is increasingly inter-disciplinary
- Need help in information exchange
- If it is not available to a computer then data is essentially lost

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

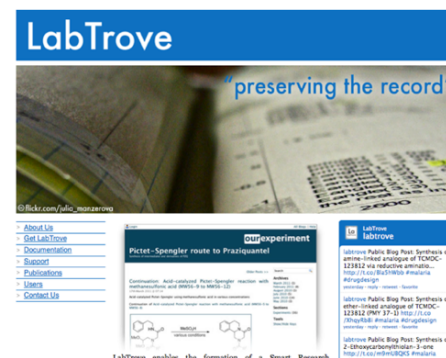
Archiving of data

- 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/regenesi/pictures>

The Trove Software



www.labtrove.org

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.



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 (1)
Lab Book Ref
JRH4712-63 (1)
JRH4712-64 (2)
JRH4712-66 (1)

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

22nd January 2007 @ 11:57

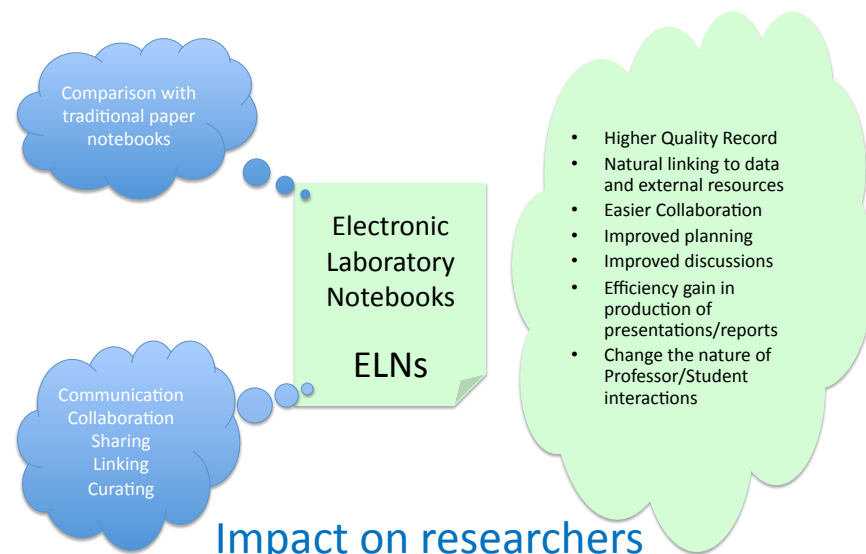
Lab Book Ref: jrh4712-89
Sample Parent: jrh4712-80, blue
Sample Parent2: jrh4712-80, white
Digestions were set up as follows:

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

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
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December 2006 (11)
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JRH4712-76 (1)
JRH4712-77 (1)
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JRH4712-87 (1)
JRH4712-88 (1)
Product
JRH4712-74 (1)
JRH4712-76 (1)
JRH4712-76a (1)



Impact on researchers

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BlogMyData
the open source blog for data scientists

HIGEM Blog

Blog for the HIGEM community

Testing POI works

27th August 2016 @ 13:40

```
Virtype rstack@iplshimont  
RegionName=HIGEM_POI21_7548151_10(18.5667)  
Dataset HIGEM_XRPR_MONTHLYMEAN  
Variable= temp  
Conventions CF-1.4  
Variable=Temperature COfi Temperature:  
Variables= degC  
File: POLYCNM121_7548151_10.689795.95.625 -15.689795.95.625 8.580213.13.10917  
6.509222.13.10917 -15.689795  
CR: EPSG:4326  
Time: 2015-06-28T16:00:00Z  
CalendarSystem: 360 Day  
Dimension: 1.00000010078683  
DimensionUnits:  
DimensionPositive: down
```

Isolated test suite for BlogMyData > HIGEM XRPR Monthly mean > Ochi Temperature.
New color scale from min to max
Color: 1.0000000000000000 to 1.0000000000000000

The figure displays a spatial visualization of temperature data. The vertical axis represents temperature in degrees Celsius, with labels at 1.0, 5.67, 18.88, and 19.13. The horizontal axis is labeled "testing POI works". The map shows a gradient of colors from blue at the bottom to red at the top, indicating increasing temperature. A yellow circle is positioned on the left side of the map, highlighting a specific point of interest.

HIGEM aims to promote e-Science methods in the environmental science community by developing new projects with collaborators in academia, government agencies as well as the public and industry. These projects will showcase the great potential of e-Science to be a useful method that environmental scientists in many disciplines can use in their everyday research. Tasks that were previously off-line and time-consuming, such as sharing and working with very large data sets, can be made much more efficient.

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October 2013

(September 2013) 2

August 2013 6

Sections

[about\(2\) \(13\)](#)

Virttype

[Stacking OGI](#)

[StackingAmplitude \(2\)](#)

[Animation \(5\)](#)

Dataset

[HIGEM XRPR MONTHLYMEAN \(13\)](#)

VariableTransformation

[Ochi Temperature\(8\)](#)

[Ochi Salinity \(2\)](#)

[Density \(3\)](#)

CalendarSystem

[360 Day \(1\)](#)

DevEolutions

[e \(12\)](#)

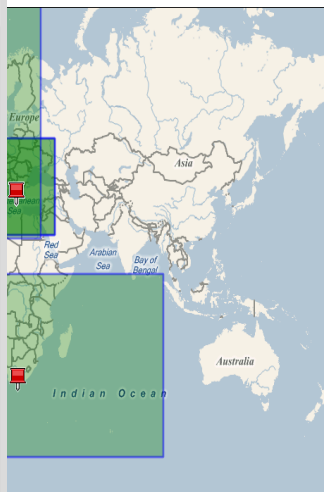
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[issues \(3\)](#)

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Nature Chemistry

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1.5 GB requirements

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Forget Apple Pay, The Masters of Mobile Payments to Starbucks | WIRED

From [The New York Times](#) via [Twitter](#)

"At Starbucks, 18 percent of US transactions took place via mobile payment app. For other major retailers per year, compare that figure to Google's book that Apple Pay alone in 1 million stores can ring in the first three days after launch."

[Jeremy Fay's insight](#)
[coffee leads the way](#)

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Hacker Lexicon: What is Homomorphic Encryption? | WIRED

From [The New York Times](#) via [Twitter](#)

"Homomorphic encryption is a method for securing data while performing just with the Turing Award. It could make sensitive information more secure for its transmission."

[Jeremy Fay's insight](#)
[too much will be possible \(when this becomes a reality\)](#)

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Wi-Fi hotspot for every 150 people

From [The New York Times](#) via [Twitter](#)

"5.6 GHz
satellite"

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New Money Paper

Free report: A look at the ROI of content creation for SMBs

Download [Scoop's](#) 2014 analysis of small businesses using content creation as a part of their marketing mix

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Fossil fuels must go by 2100 - IPCC



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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.

_____ available at this time.

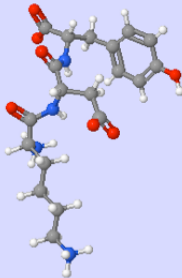
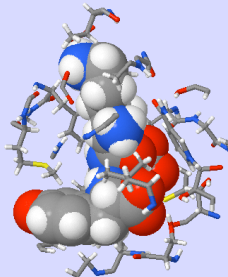
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Molecules - My Molecules

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Citizen Science



Foldit

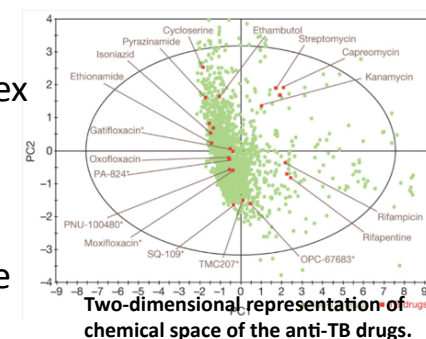


Kaggle

Big Data

- Chemistry we have -
- Big, Broad, Bothersome, & Brocken,*

High Dimensional, Heterogeneous, Complex Data on an uncertain landscape as we still do not have a really good grasp of Chemical Space



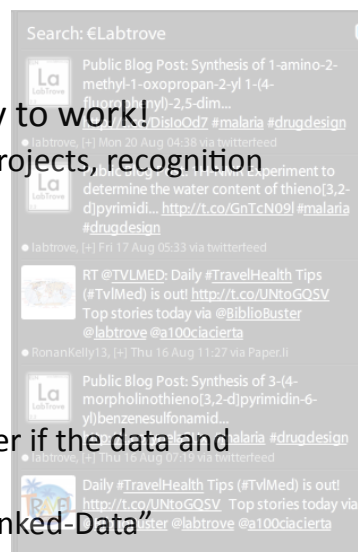
Two-dimensional representation of chemical space of the anti-TB drugs.

Open Notebook Science

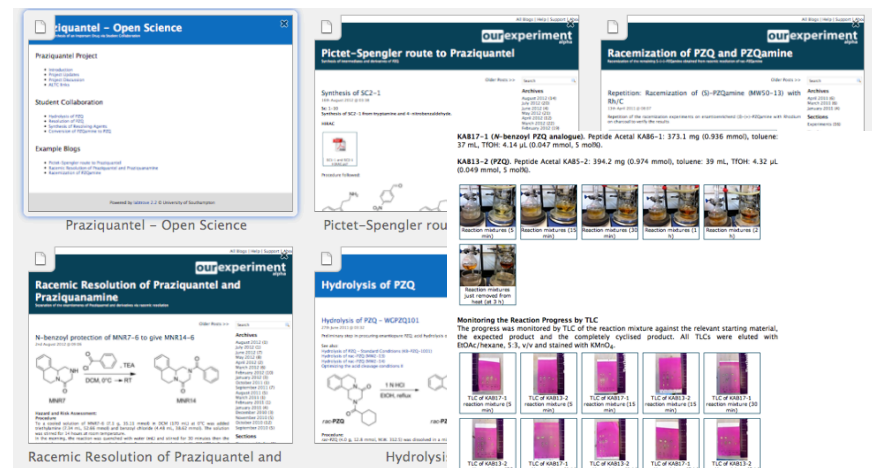
- Certainly not always the way to work!
 - IPR, Commercial, long term projects, recognition issues, etc

*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



LabTrove -> RSS -> Email / Twitter

IFTTT

My RecipesBrowseChannelsjgfrey

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.

Create a Recipe

Filter

if  then 

if new feed item from http://xray.ocr.soton.ac.uk/feeds/xray_group/u/ld/2e675a007d7c25e25a4e672d1954b842?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

DataCite DOI

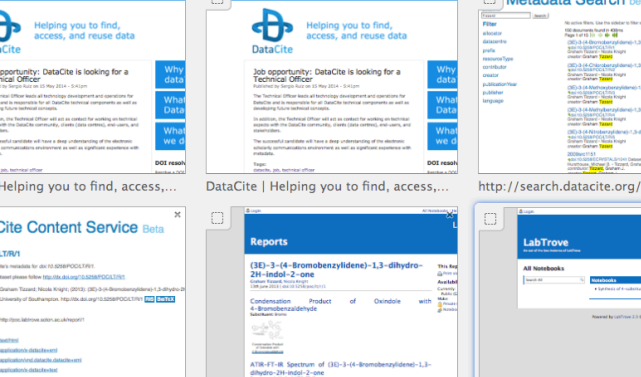


Figure 1 displays a series of screenshots from the DataCite website, illustrating its various features and services. The screenshots are arranged in a grid format, showing the homepage, job opportunities, metadata search, content service, reports, and lab tools.

The first row shows the DataCite homepage, featuring the logo and navigation menu. The second row displays a job opportunity for a Technical Officer, highlighting the company's commitment to diversity and inclusion. The third row shows the Metadata Search page, which allows users to search for datasets and publications. The fourth row displays the DataCite Content Service, which provides access to a wide range of research data. The fifth row shows the Reports page, which provides information on the company's financial performance and other key metrics. The sixth row displays the LabTools page, which provides information on the company's laboratory equipment and services.

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



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

*In times of change it is even more important to
bring dissemination in to the lab...*

**DISSEMINATION IS PART OF THE
RESEARCH**

**Change in the whole way we design and
build experiments**



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

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