



Digital Chemistry

Reducing and Managing Uncertainty

Chemistry 2.0 (or 3.0)





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

A Chemist's Digital Aura

The collage displays four digital profiles for Jeremy G. Frey:

- Google Scholar Citations:** Shows a profile for Jeremy G. Frey at the University of Southampton, with 2997 citations and a bar chart of citation trends from 2006 to 2014. A list of publications is provided, including "Quantities, units and symbols in physical chemistry" (934 citations, 2007) and "Infrared predissociation spectra of water dimer in a supersonic molecular beam" (150 citations, 1984).
- Impactstory:** Displays 143 articles with 102.4k impressions and 3.4k views. Articles include "Laboratory notebooks in the digital era: the role of ELNs in record keeping for chemistry and other sciences" and "Towards predictable transmembrane transport: QSAR analysis of amino binding and transport".
- Atlassian Stash:** A GitHub-like profile for Jeremy Frey, showing a bio, location (Southampton, United Kingdom), and a bioRxiv preprint titled "Science Ajar: The future of research: are you ready?".
- LinkedIn:** A professional profile for Jeremy Frey, Head of Computational Systems Chemistry at the University of Southampton, with 500+ connections and a detailed background section.

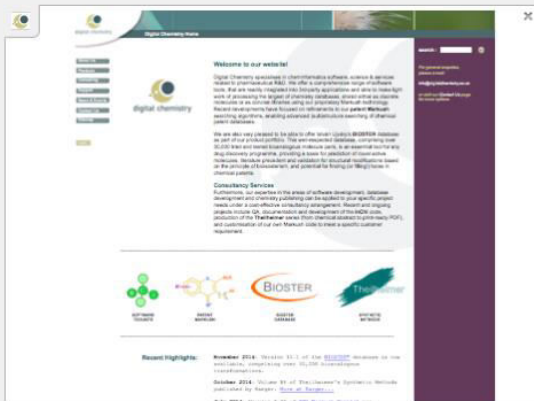
Jeremy G. Frey – Google Scholar Citations

Impactstory: Jeremy Frey

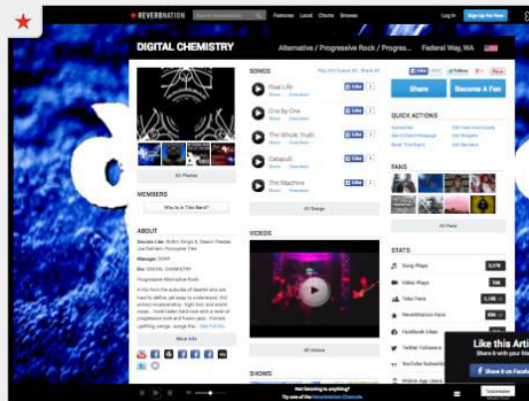
Jeremy Frey, Professor at Uiveristy of south...

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Digital Chemistry - Home



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Welcome to the Chemical Education Digital Library



Event details: DNA-Based Nanotechnology: Digital Chemistry - p...



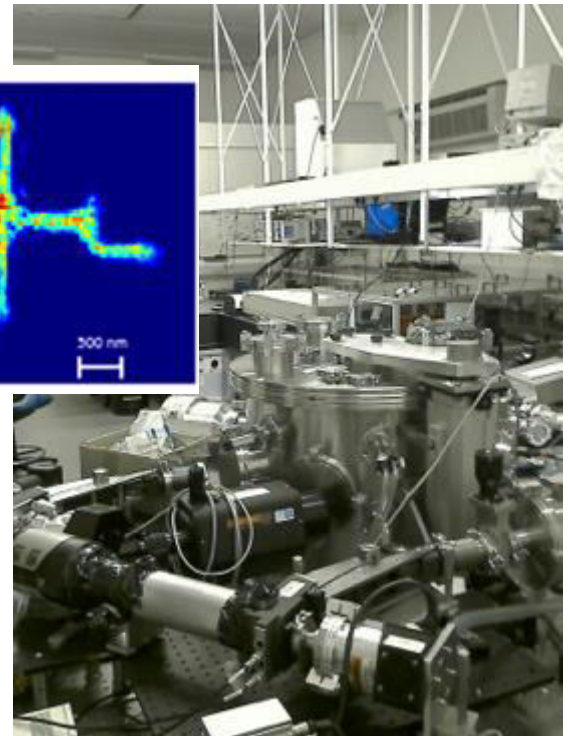
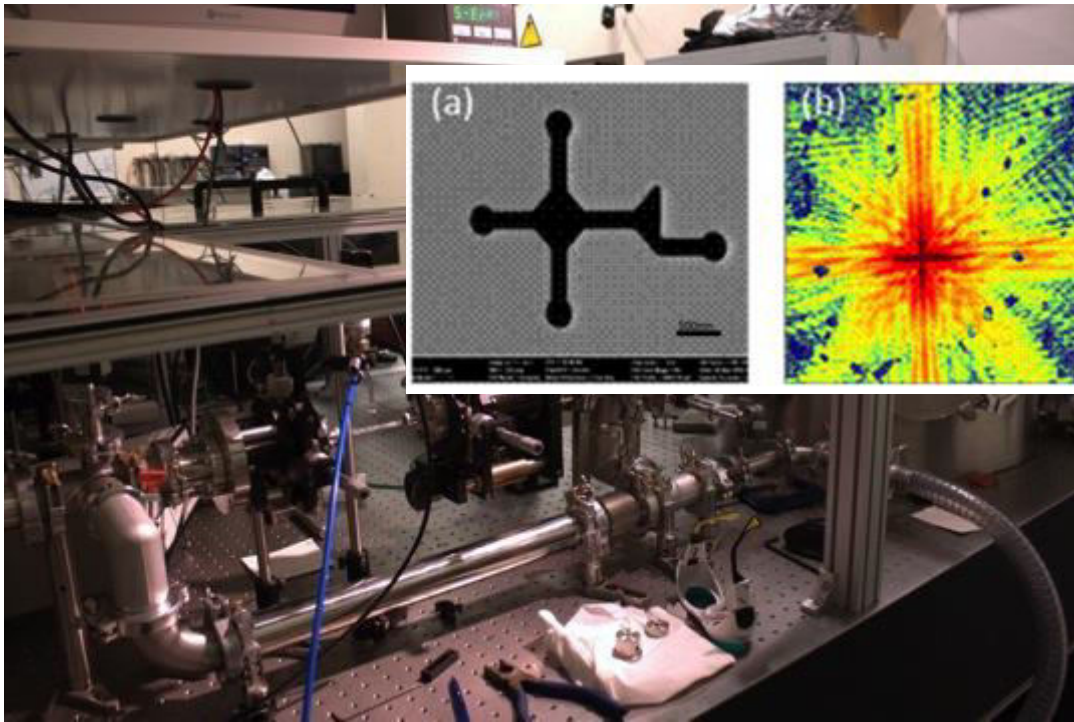
Digital Specialty Chemicals

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





UNIVERSITY OF Southampton

UltraFast Xray Group

<< Next Post Previous Post >> Search


Reconstructing the new data

3rd August 2011 @ 22:52

Just a quick post to show some pictures from the reconstructions of the latest data and update everyone on progress.

Looking at data taken on 2nd August – the old 2um sample taken with a single wavelength. The diffraction patterns look v clean, with good detail right out to the edge – haven't worked out the resolution yet.

Tried to get Ben's CDI routine working, but it broke badly, and I couldn't fix it immediately, so I went back to my old routines (from 2 years ago! can't believe it's been that long) and got '106.m' working. This is running on Boxer under Windows, but not using anything clever.



1000_recon001.png

This one is a very plain HIO reconstruction, 1000 iterations after binning the data to 512x512. Shrinkwrapping every 100 (I think – notes at work right now). You can see that it reconstructs beautifully, and this happens every time – no need for multiple phases to get it to work.

(Once I'd remembered to background-subtract properly, of course – before that it all failed

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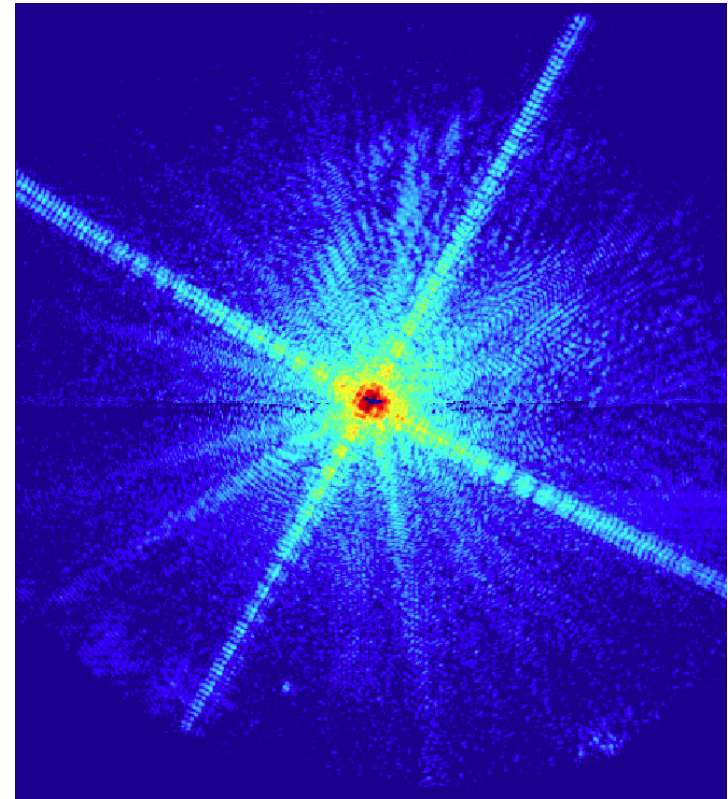
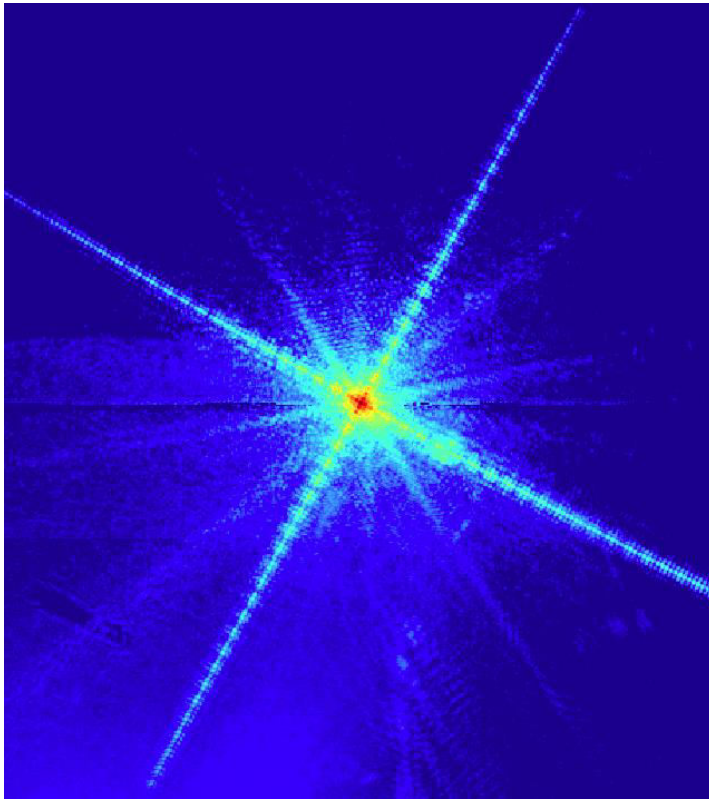
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Timeline

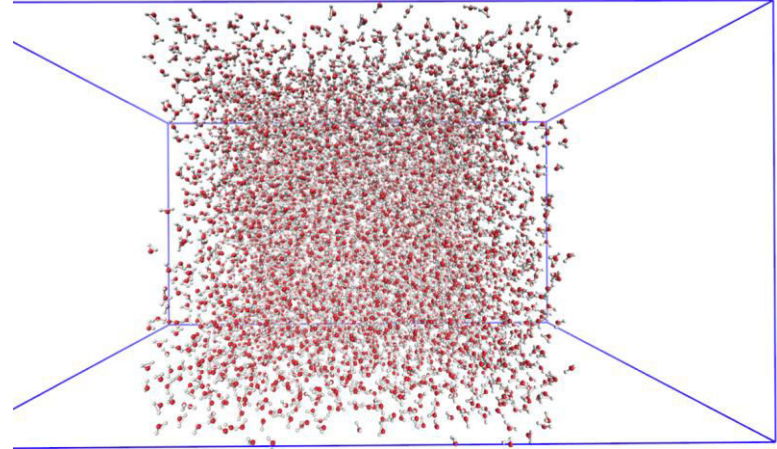
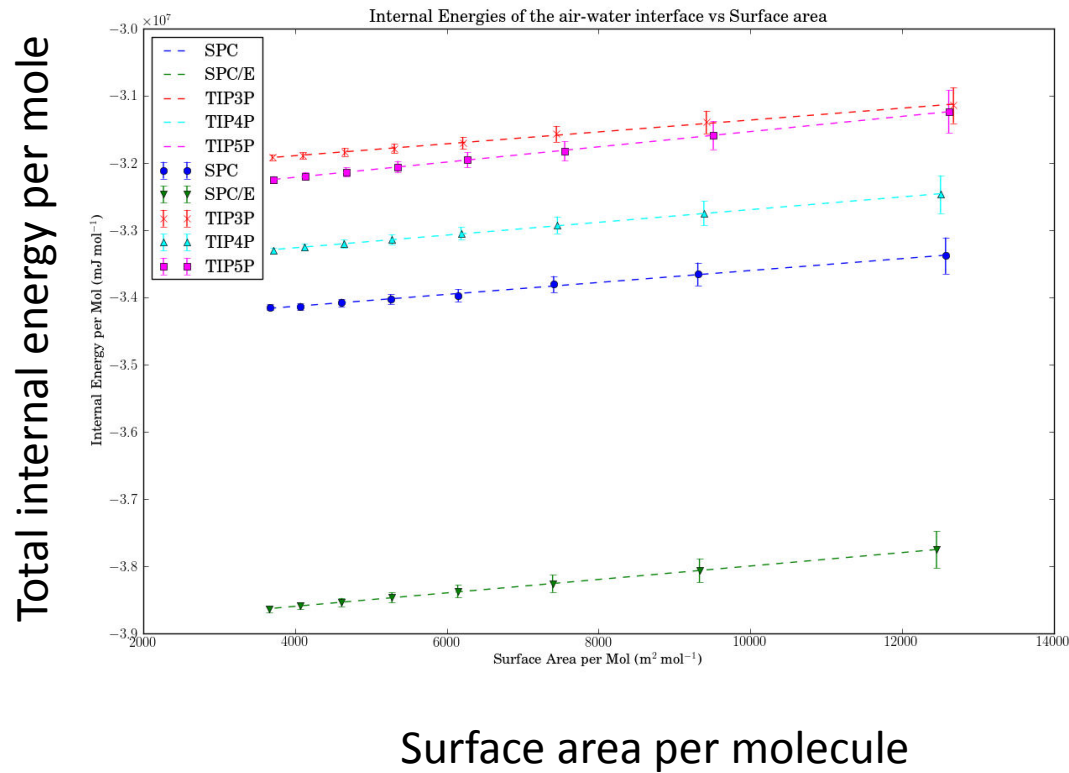
- 1-SWAMP
- 2 micron diffraction pattern
- SIN AI
- Microscope images
- Change to Matlab licensing on Iridis
- Hello!
- Zr and Nb data
- Grid diffraction through focus
- 2 micron fib sample maps
- Micro and Nano sensors workshop
- Hippocampal sample progress
- GPU coding initial work for SYMBIOSIS
-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

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.

Lyons Electronic Office (LEO) 1951

Information Transformation



In October 1947, the directors of J. Lyons & Company, a British catering company famous for its teashops but with strong interests in new office management techniques, decided to take an active role in promoting the commercial development of computers.

In 1951 the LEO I computer was operational and ran the world's first regular routine office computer job.

The company LEO Computers Ltd was formed in 1954.

Reducing Uncertainty

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



Collaboration

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



Related links

[Open Data White Paper: Unleashing the Potential](#)

Open Data White Paper and Departmental Open Data Strategies

28 June 2012

Open Data White Paper
Replay

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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 to public services and for economic growth. It will also bring opportunities for more public engagement with research and downloading below, along with an executive summary.

The internet has brought much better access to research for the public and business. 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 internet is to create a worldwide open access regime. The key to this is 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.

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.

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.

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- 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

Areas for action

The report highlights the need for the report to be widely accessible and to be discussed with the public and media. The following areas for action are identified:

- Scientists need to be more open in their communication with the public and media
- Greater recognition needs to be given to the value of open access to research data
- Common standards for sharing information are required to make it widely usable

Intelligent Open Access to Data



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

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'Show Your Working': What 'ClimateGate' means



VIEWER
Mike Hulme

The "ClimateGate" affair documents hacked or leaked climate research institute web. But what does it mean for Hulme and Jerome Ray concerted effort to explain understanding the process scientists.

As the repercussions of ClimateGate reverberate the virtual community of citizens, we believe it is a important and urgent to report what this moment is telling about the practice of science the 21st Century.



Byte Size Biology

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

StructureGate

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Home > Science, Structural biology > Structuregate?

Structuregate?

December 10th, 2009

Go to comments Leave a comment

The University of Alabama at Birmingham issued a statement last week asking that 11 structures be removed from the Protein Data Bank as their use might constitute "misuse". Very little detail was given as to why the structures are tied to the report by the Bin. The structures' PDB IDs are 1CHW, 1DF9/2QID, and still in the database.



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CRU Scientific Assessment Panel announced

Mon, 22 Mar 2010

Lord Oxburgh FR5, a former chair of the Lords Select Committee on Science and Technology, is to chair an independent Scientific Assessment Panel to examine important elements of the published science of the Climatic Research Unit (CRU) at the University of East Anglia.

His appointment has been made on the recommendation of the Royal Society, which has also been consulted on the choice of the six distinguished scientists who have been invited to be members of the panel.

The panel will have access to any publications or materials it requests, and all information considered will be listed in the Report. The University, in consultation with the Royal Society, has suggested that the panel looks in particular at key publications, from the body of CRU's research referred to in the UEA submission to the Parliamentary Science and Technology Committee.

Announcing the appointment, Prof Trevor Davies, the University's Pro-Vice-Chancellor for Research, said: "CRU's scientific papers have been examined by scientists from other institutions through the peer review process before being accepted for publication by international journals. We have no reason to question the effectiveness of this process. Nevertheless, given the concerns about climate research expressed by some in the media, we decided to augment the Muir Russell review with an independent assessment of CRU's key publications in the areas which have been most subject to comment."

"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 great 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,

The University Collaboratory structure files publications various scientific Allegations of protein structure scientific interest Department of no conflicting of the available s.sodahead.com...



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

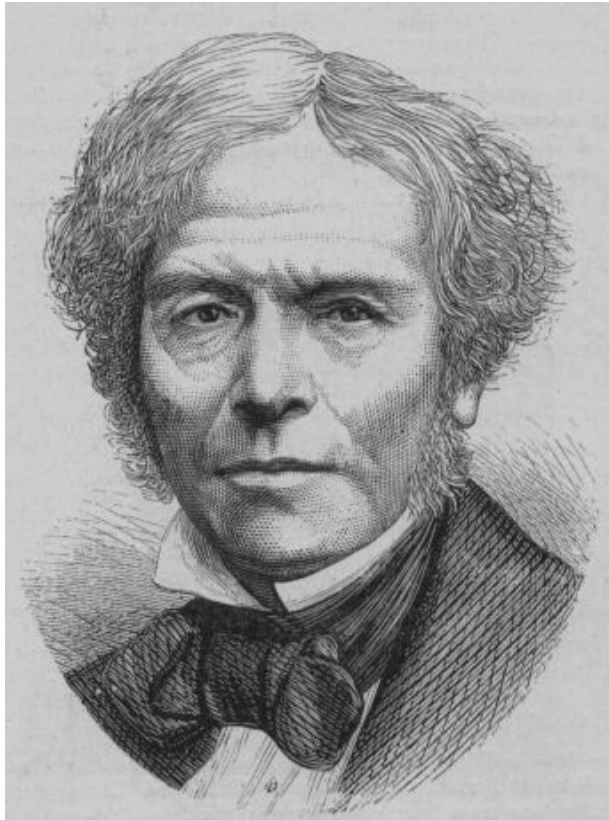
What is the story? What is the why?

THE RESEARCH 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'



If only I knew exactly how she did this experiments

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

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

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

Typical Laboratory

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>

The Trove Software



LabTrove

“preserving the record”

© flickr.com/julia_manzerova

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our experiment

Pictet-Spengler route to Praziquantel

Continuation: Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MW56-9 to MW56-12)

All acid-catalyzed Pictet-Spengler reactions using methanesulfonic acid in various concentrations

Continuation of Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MW56-9 to MW56-12)

C1=CC=C(C=C1)N(C)C(=O)O + C1=CC=C(C=C1)N(C)C(=O)O >> C1=CC=C(C=C1)N(C)C(=O)N(C)C(=O)O

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Transformation of plasmid JRH4712/66 into BW25141 by electroporation

11th December 2006 @ 14:31

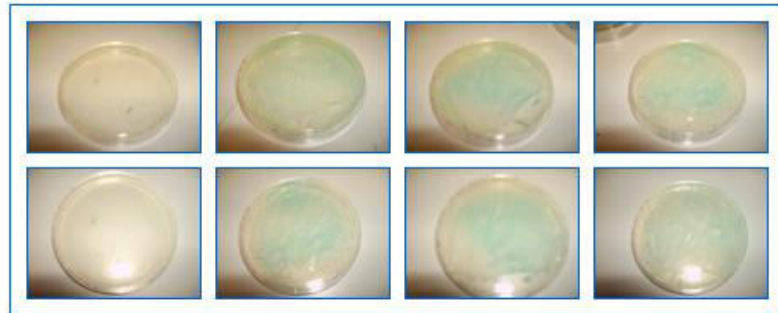
Transformations were set up according to the following protocol: LB Ampicillin arabinose plates and SOC medium were warmed to 37 °C briefly before the arabinose plates were spread with X-glu (80 µL, 1:1 X-glu and LB) and allowed to continue warming.

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)
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	-	-	-	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

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Lab Book Ref

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

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

Comparison with
traditional paper
notebooks

Electronic
Laboratory
Notebooks

ELNs

Communication
Collaboration
Sharing
Linking
Curating

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

Impact on researchers

HiGEM Blog

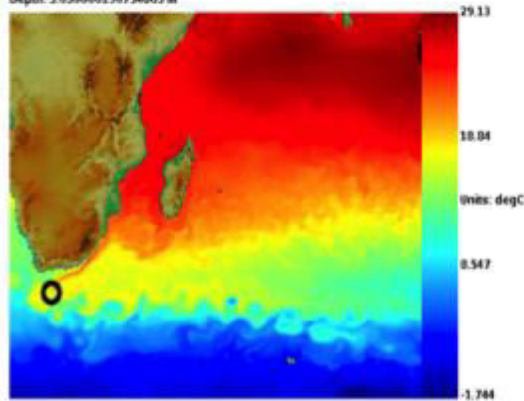
Blog for the HiGEM community

Testing POI works

27th August 2010 @ 13:40

Viztype: staticMapWithPoint
RegionofInterest: POINT(21.794815 -38.095867)
Dataset: HiGEM_XBYLR_MONTHLYMEAN
Variableid: temp
Conventions: CF-1.4
Variablestandardname: OClr/ Temperature.
Variableunits: degC
Box: POLYGON((13.359375 -55.689785,95.625 -55.689785,95.625 8.580235,13.359375 8.580235,13.359375 -55.689785))
Crs: EPSG:4326
Time: 2010-08-16T00:00:00.000Z
Calendarsystem: 360_day
Elevation: 5.050000190734863
Elevationunits: m
Elevationpositive: down

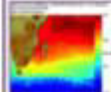
Godiva2 test site for BlogMyData > HiGEM XBYLR Monthly means > OClr/ Temperature.
 Time: 2010-08-16T00:00:00.000Z
 Depth: 5.050000190734863 m



Testing POI works

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

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M (13)

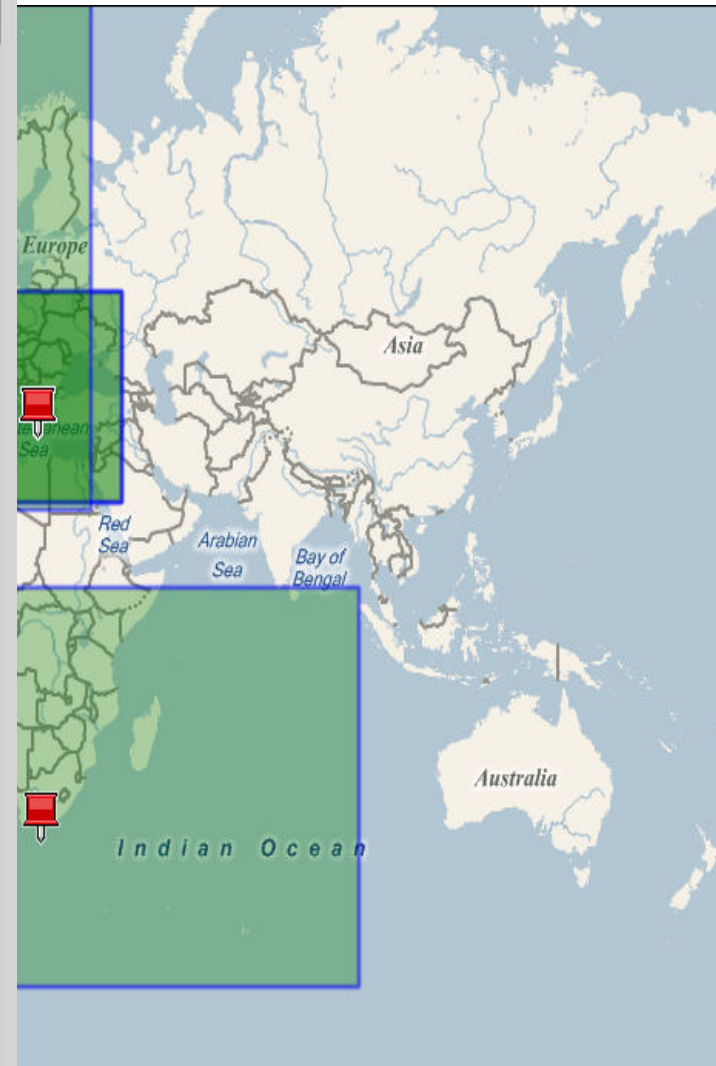
Elevationpositive

Down (13)

Tools

Show/Hide QR Code
 Show/Hide Keys

BlogMyData Project - Godiva



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

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Scoped by Jeremy Frey
onto IT as a Utility Digital Economy Network

Forget Apple Pay. The Master of Mobile Payments Is Starbucks | WIRED

From [www.wired.com](#) - November 3, 7:38 PM

"At Starbucks, 16 percent of US transactions took place via a mobile device—about 7 million mobile payments per week. Compare that figure to Cook's boast that Apple Pay saw 1 million credit cards registered in the first three days after launch."

Jeremy Frey's insight:
coffee leads the way

Scoped by Jeremy Frey
onto Atmospheric Chemistry

Fossil fuels must go by 2100 - IPCC

From [www.bbc.co.uk](#)

Scoped by Jeremy Frey
onto IT as a Utility Digital Economy Network

Hacker Lexicon: What Is Homomorphic Encryption? | WIRED

From [www.wired.com](#) - November 3, 7:42 PM

"Homomorphic encryption is a method for securing data whose inventor just won the MacArthur Genius Award. It could make sensitive information more secure, but it's incredibly difficult."

Jeremy Frey's insight:
So much will be possible if/when this becomes a reality

Scoped by Jeremy Frey
onto IT as a Utility Digital Economy Network

Wi-fi hotspot for every 150 people

From [www.bbc.co.uk](#) - November 3, 1:50 PM
society

New White Paper

What is the place of curation in SMBs' content marketing mix?
A report by [Scoop.it](#)

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

Download Scoop.it's 2014 analysis of small businesses using content curation as a part of their marketing mix today.

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My Curated Topics

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100 suggestions

[IT as a Utility Digital Econ...](#)
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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.



Home

CCDC

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e-Malaria

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Schools

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Molecules - My Molecules

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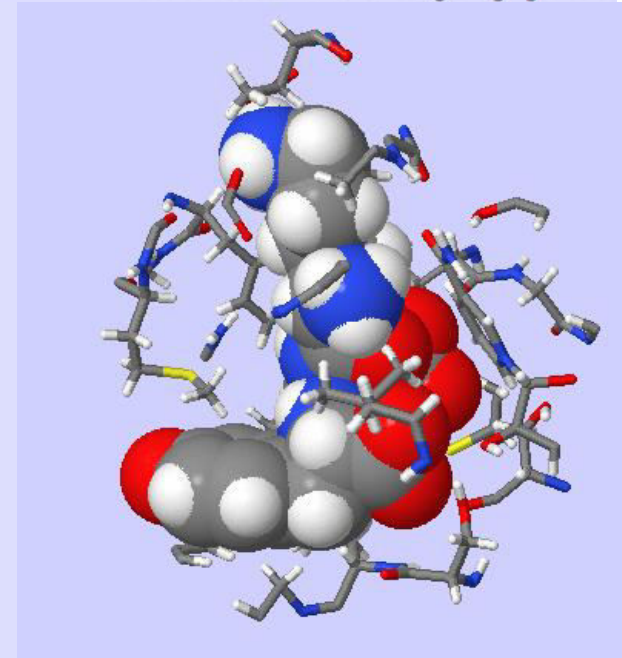
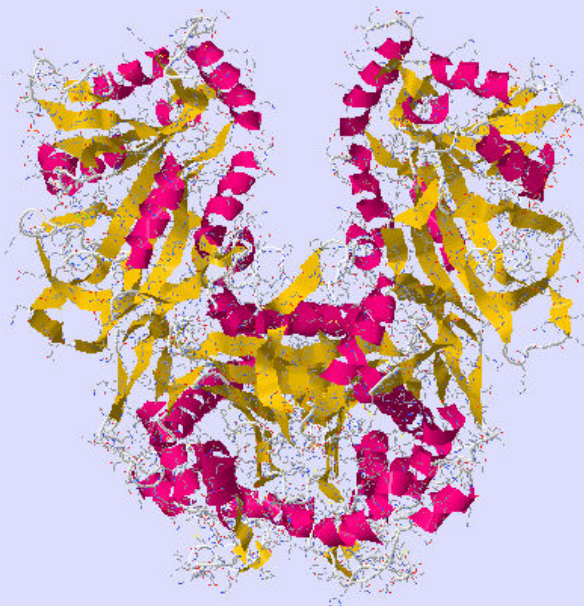
available at this time.

Sort By

ise. As resistance to existing drugs grows ar



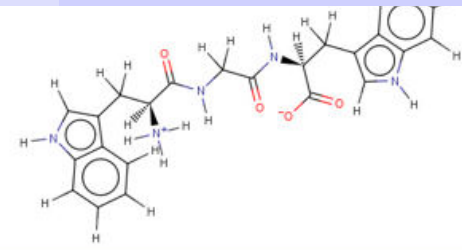
Jmol



- Malaria
- [Introduction](#)
- [Symptoms](#)
- [Treatments](#)
- [Prevention](#)
- [Target](#)

- Threonine thr t
- Tryptophan trp w
- Tyrosine tyr y
- Valine val v
- Methionine met m

- Malaria
- [Introduction](#)
- [Symptoms](#)
- [Treatments](#)
- [Prevention](#)
- [Target](#)
- Chemistry
- [Bonding](#)
- [Hydrophilicity](#)
- [Structure](#)
- [Proteins](#)



Citizen Science

The screenshot shows the Foldit website interface. At the top, there is a green header with the Foldit logo and navigation links for PUZZLES, BLOG, CATEGORIES, FEEDBACK, GROUPS, FORUM, PLAYERS, WIKI, RECIPES, FAQ, ABOUT, CONTESTS, and CREDITS. The main content area features a large 3D protein structure puzzle with a text box that says "Click to learn how you contribute to science by playing Foldit." Below this is a "HANDCRAFTER" banner for a new scientific discovery game. The right sidebar contains a "GET STARTED: DOWNLOAD" section with buttons for Win Beta, Mac Beta, and Linux Beta, along with links for new users and educators. There is also a search bar, a "RECOMMEND FOLDIT" form, and a "USER LOGIN" section with fields for username and password. At the bottom, there is a table of "SOLOISTS" and "TOP NEW USERS".

What's New

Help us to solve a Vascular endothelial growth factor protein!

Vascular endothelial growth factor (VEGF) is a protein released to trigger new blood vessels to form. This is important in embryonic development and when healing from cuts and damage, but it can also be hijacked by cancer cells to trick the body into providing extra blood vessels (angiogenesis).

Puzzle 1012 comes from the VEGF receptor (type 1). The receptor forms a membrane dimer, with an extracellular part that binds VEGF and an intracellular kinase domain which is responsible for signaling. The extracellular portion consists of seven Immunoglobulin-like (Ig) domains. This puzzle consists of the sequence for domain 6. Some experimental data has been collected for the VEGF receptor, but it hasn't yet lead to a finished structure. The hope is that if you can help us find near-native solutions then your Foldit predictions can be used to improve the structure. That in turn could lead to a better understanding of angiogenesis and eventually to new anti-cancer treatments.

Please try out the first puzzle for this unsolved protein [here](#).

(Posted by [beta_helix](#) 121 3960 | Wed, 11/12/2014 - 20:18 | 0 comments)

Puzzle 1011 Issues

HEADS UP: Puzzle 1011 will be closing and we'll be posting a different target today - turns out the target was the same as 1008! Big thanks for the sharp eyes in the community who pointed that out to us. We are sorry for any hassle this may cause you.

SOLOISTS	EVOLVERS	GROUPS	TOPICS
PLAYER	PUZZLE	SCORE	
deLaCeba 121	102	1013: Revisitin...yle	9,874
nicobul 54	10	1012: Unsolved ...yle	8,445
BitSpawm 62	2	1010: Abeta Bin...ign	10,335
sommerr 121	1340	Beginner Puzzle...ign	8,986
jetoddard 121	1299	Beginner Puzzle...ity	14,438
heterologicaln... 121	551	Beginner Puzzle...nls	9,242
Maru67 121	247	Beginner Puzzle...zle	8,694
rjsthehird 121	210	Beginner Puzzle...ign	11,133
jetoddard 121	1299	Beginner Puzzle...yle	8,660
		FULL	

TOP NEW USERS

- yogenzaga
- hildred

Foldit

The screenshot shows the Kaggle website interface. At the top, there is a dark header with the Kaggle logo and buttons for "Start competing" and "Login". The main content area features a large graphic with the text "The Home of Data Science" and a list of services: ENERGY INDUSTRY SPECIALISTS, PREDICTIVE MODELING SOLUTIONS, COMPETITIONS FOR DATA SCIENTISTS, TUTORIALS, UNIVERSITY COMPETITIONS, and DATA SCIENCE JOBS BOARD. Below this is a red banner with the text "HIRING DATA SCIENTISTS? POST TO OUR JOBS BOARD". The bottom section is blue and contains two columns: "FOCUSED ON ENERGY" with an icon of a factory and a brain, and "COMPETITIVE ANALYTICS" with an icon of a brain and a flag. Each column has a "Find out more" or "Host a competition" button.

The Home of Data Science

ENERGY INDUSTRY SPECIALISTS • PREDICTIVE MODELING SOLUTIONS •
COMPETITIONS FOR DATA SCIENTISTS • TUTORIALS •
UNIVERSITY COMPETITIONS • DATA SCIENCE JOBS BOARD

HIRING DATA SCIENTISTS? POST TO OUR JOBS BOARD

FOR CUSTOMERS

FOCUSED ON ENERGY

The Energy Industry uses our expertise in machine learning & big data to drive high-stakes decisions.

[Find out more >](#)

COMPETITIVE ANALYTICS

For any industry, we tap the world's largest community of data scientists to solve your data problem.

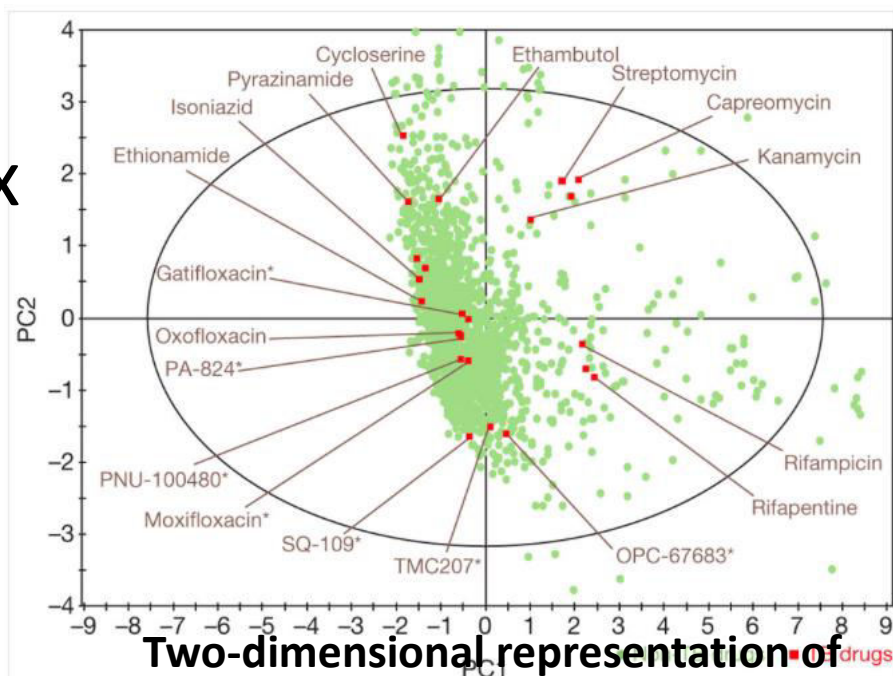
[Host a competition >](#)

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

Praziquantel – Open Science
Read all an experiment blog by student Collaborators

Praziquantel Project

- Introduction
- Project Goals
- Project Discussion
- ATC Codes

Student Collaboration

- Hydrolysis of PZQ
- Resolution of PZQ
- Synthesis of Racemizing Agents
- Conversion of PZQamine to PZQ

Example Blogs

- Pictet-Spengler route to Praziquantel
- Kinetic 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

19th 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-LIC-PZQamine obtained from kinetic resolution of PZQamine

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

13th April 2012 @ 08:07

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)

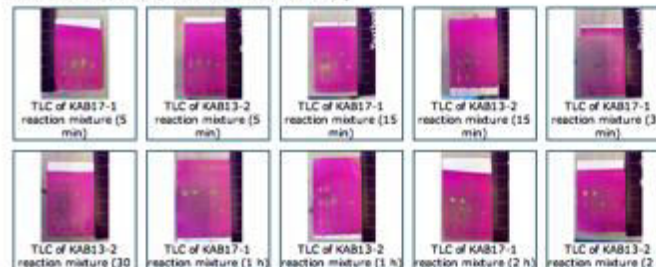
KAB17-1 (N-benzoyl PZQ analogue). Peptide Acetal KAB6-1: 373.1 mg (0.936 mmol), toluene: 37 mL, TFOH: 4.14 μ L (0.047 mmol, 5 mol%).

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 (0.1 g, 0.13 mmol) in DCM (170 mL) at 0°C was added triethylamine (0.34 mL, 0.26 mmol) and benzoyl chloride (0.48 mL, 0.26 mmol). The solution was stirred for 14 hours at room temperature.

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

Archives:

- August 2012 (1)
- July 2012 (2)
- June 2012 (1)
- May 2012 (1)
- April 2012 (2)
- March 2012 (2)
- February 2012 (1)
- January 2012 (1)
- December 2011 (1)
- November 2011 (1)
- October 2011 (1)
- September 2011 (1)
- August 2011 (2)
- July 2011 (2)
- June 2011 (1)
- May 2011 (1)
- April 2011 (1)
- March 2011 (1)
- February 2011 (1)
- January 2011 (1)
- December 2010 (1)
- November 2010 (1)
- October 2010 (1)
- September 2010 (1)

Sections:

Racemic Resolution of Praziquantel and

Hydrolysis of PZQ

Hydrolysis of PZQ – WGPZQ101

17th June 2012 @ 09:30

Preparatory step in producing enantiomeric PZQ acid hydrolysis of

See also:

- Hydrolysis of PZQ – Standard Conditions (00-002-1001)
- Hydrolysis of ac-PZQ (0002-110)
- Hydrolysis of ac-PZQ (0002-110)
- Optimizing the acid cleavage conditions 8





Procedure:

rac-PZQ (4.0 g, 12.8 mmol, 90% (12.5)) was dissolved in a mL

Hydrolysis

LabTrove -> RSS -> Email / Twitter

The screenshot shows the 'My Recipes' page in LabTrove. At the top, there is a navigation bar with 'My Recipes', 'Browse', 'Channels', and a user profile 'jgfrey'. Below this is a header for 'My Recipes' with tabs for 'Personal', 'Shared', and 'Favorites'. A status indicator shows '2 Personal Recipes, 2 turned on'. A blue button labeled 'Create a Recipe' is visible. Below the header, there is a 'Filter' dropdown. The main content area displays two recipes:

- Recipe 1:** 'if  then '. Description: 'If new feed item from http://xray.orc.soton.ac.uk/feeds/xray_group/uid/2e575a007d7c25e2e54e672d1954b842?withcomments, then send me an email at'. Status: 'created less than a minute ago', 'never triggered'. Controls: Power, Refresh, Delete, Play.
- Recipe 2:** 'if  then '. Description: 'RSS to Twitter'. Status: 'created February 25, 2014', 'last triggered April 02, 2014', 'triggered 10 times'. Controls: Power, Refresh, Delete, Play.

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

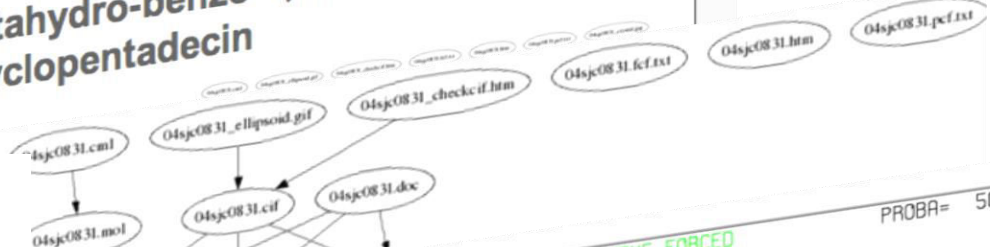
InChI=1/C1414/h1-4H,5-

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Controll
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



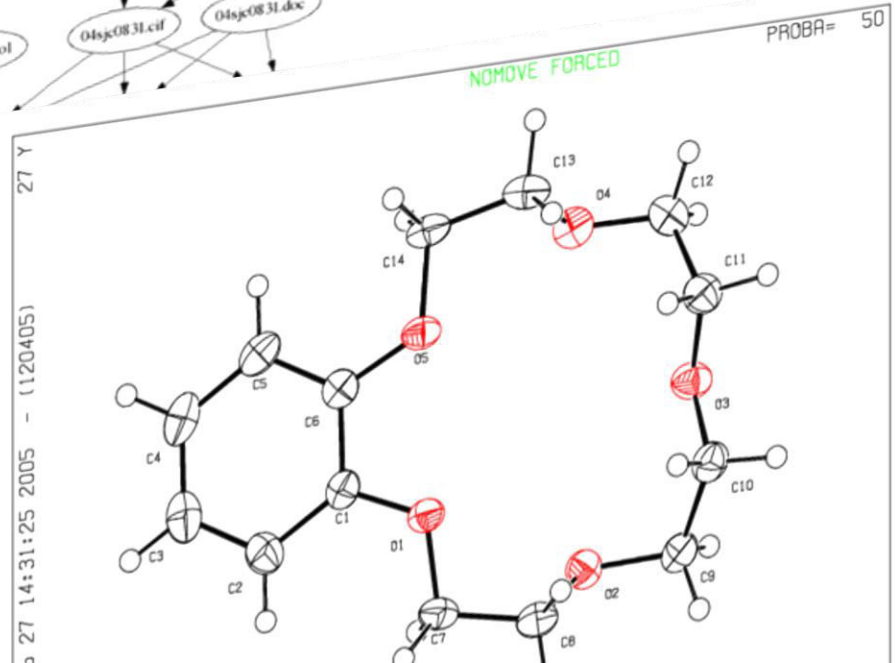
Graph/Network provides intuitive navigation

Depositor
Structure al
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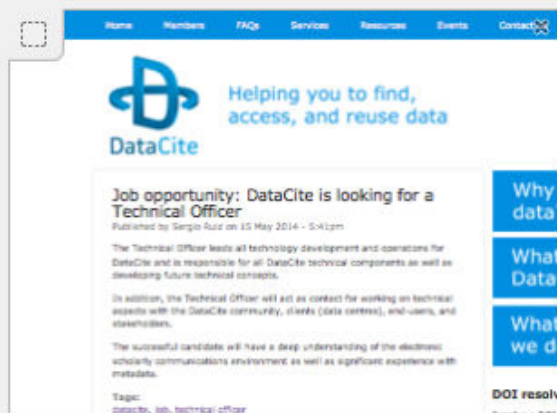
Creator: CO
Creator: Hur
Date: 200

Stages (10)

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



DataCite DOI



Home Members FAQs Services Resources Events Contact

DataCite Helping you to find, access, and reuse data

Job opportunity: DataCite is looking for a Technical Officer
Published by Sergio Ruiz on 15 May 2014 - 5:41pm

The Technical Officer leads all technology development and operations for DataCite and is responsible for all DataCite technical components as well as developing future technical concepts.

In addition, the Technical Officer will act as contact for working on technical aspects with the DataCite community, clients (data centers), end-users, and stakeholders.

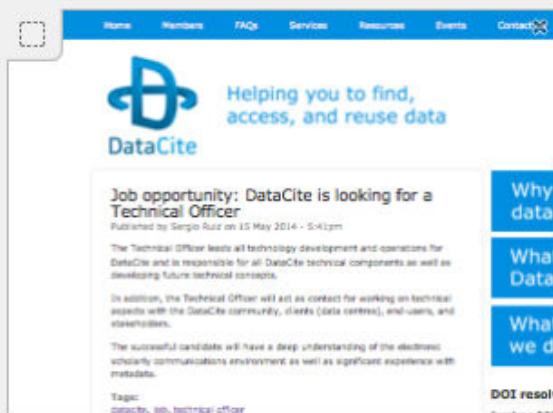
The successful candidate will have a deep understanding of the electronic scholarly communications environment as well as significant experience with metadata.

Tags: [contact](#), [job](#), [technical officer](#)

Why data
What Data
What we d

DOI resolv
Resolving a DOI

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



Home Members FAQs Services Resources Events Contact

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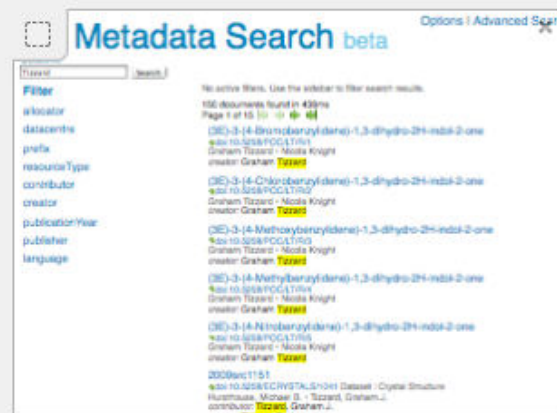
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Why data
What Data
What we d

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Resolving a DOI

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



Metadata Search beta Options | Advanced Search

Filter

150 documents found in 459ms
Page 1 of 15 (1) (2) (3) (4)

(3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one
doi:10.5258/POC/LT/R/1
Graham Tizzard - Nicola Knight
creator: Graham Tizzard

(3E)-3-(4-Chlorobenzylidene)-1,3-dihydro-2H-indol-2-one
doi:10.5258/POC/LT/R/2
Graham Tizzard - Nicola Knight
creator: Graham Tizzard

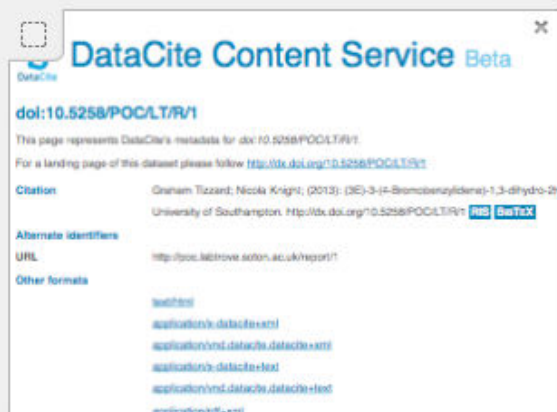
(3E)-3-(4-Methoxybenzylidene)-1,3-dihydro-2H-indol-2-one
doi:10.5258/POC/LT/R/3
Graham Tizzard - Nicola Knight
creator: Graham Tizzard

(3E)-3-(4-Methylbenzylidene)-1,3-dihydro-2H-indol-2-one
doi:10.5258/POC/LT/R/4
Graham Tizzard - Nicola Knight
creator: Graham Tizzard

(3E)-3-(4-Nitrobenzylidene)-1,3-dihydro-2H-indol-2-one
doi:10.5258/POC/LT/R/5
Graham Tizzard - Nicola Knight
creator: Graham Tizzard

DOI:10.5258/1151
doi:10.5258/1151
Crystal Structure
Huzumeike, Mutsaers B., Tizzard, Graham J.,
contributor: Graham Tizzard, Nicola Knight

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



DataCite Content Service Beta

doi:10.5258/POC/LT/R/1

This page represents DataCite's metadata for doi:10.5258/POC/LT/R/1.
For a landing page of this dataset please follow <http://dx.doi.org/10.5258/POC/LT/R/1>

Citation: Graham Tizzard, Nicola Knight, (2013). (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one. University of Southampton. <http://dx.doi.org/10.5258/POC/LT/R/1> [RIS](#) [BibTeX](#)

Alternate identifiers

URL: <http://www.labtrove.soton.ac.uk/report/1/>

Other formats

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[application/vnd.datacite+dataverse+xml](#)
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[application/vnd.datacite+dataverse+xml](#)
[application/vnd+xml](#)

10.5258/POC/LT/R/1



Reports

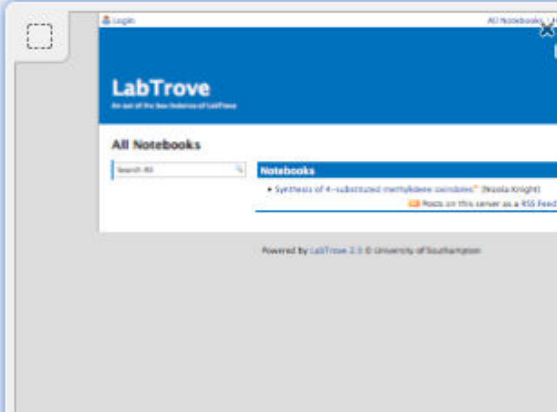
(3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one
Graham Tizzard, Nicola Knight
13th June 2013 | doi:10.5258/1151/1

This Key
Print
Availability
Curator
Public
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Private
Nobis

Condensation Product of Oxindole with 4-Bromobenzaldehyde
Substrates: Bromo

ATIR-FT-IR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one
Spectroscopic Method: ATIR-FT-IR
Substrates: Bromo
ATIR-FT-IR Spectrum of (3E)-3-(4-Bromobenzylidene)-1,3-dihydro-2H-indol-2-one

Reports



LabTrove
An app of the best resources of LabTrove

All Notebooks

Search All

Notebooks

- Synthesis of 4-substituted methylidene oxindoles* (Nicola Knight)

Posts on this server as a RSS feed

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LabTrove

We must speed up the knowledge discovery process



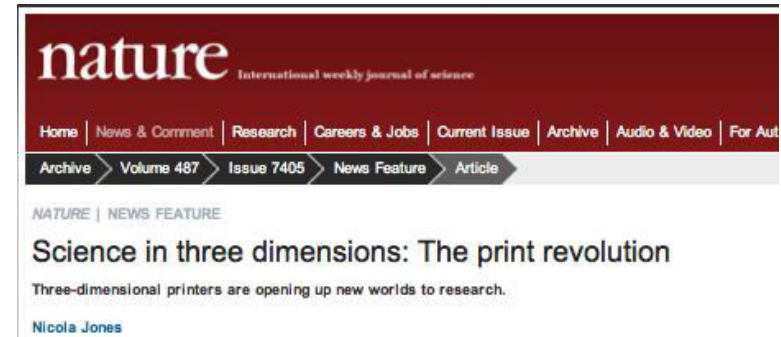
© The New Yorker collection. All rights reserved.
From *The New Yorker Book of Technology Cartoons*.

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



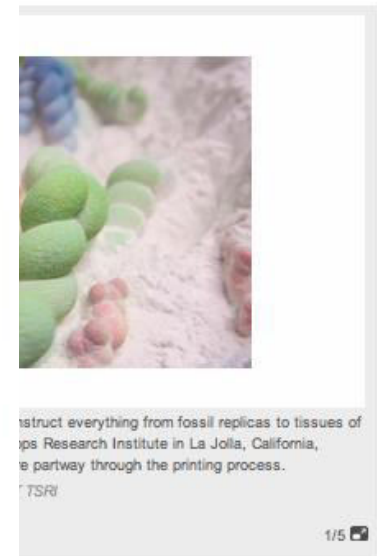
*Everything is Awesome,
Everything is cool when you're part of a team*

Change in the whole way we design and build experiments



Digital fabrication is so much more than 3D printing

By Olivia Solon | 13 March 13



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

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

**DISSEMINATION IS PART OF THE
RESEARCH**

Thank you for listening



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