

Science Ajar

How e-Science can help (more) Open Science

Jeremy G. Frey
15 March 2013



DreChem

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Talk Themes

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

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Light Microscope

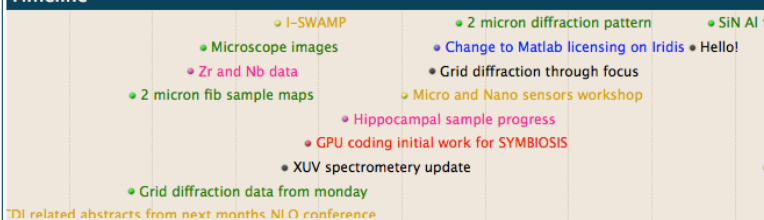
UltraFast Xray Group

<< Next Post

Previous Post >>

Search

Timeline



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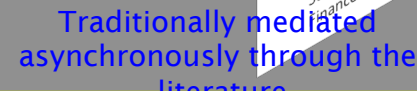
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Commercial response to governmental OA mandates



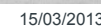


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Scientific Narratives

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'

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Scientific information supply helix

- Historically
 - Researcher → Literature → Abstraction/Search → Literature
- Currently now add for Open Notebook Science)
 - Researcher → ?Web? → Search → Researcher
 - But rarely the only dissemination route!
- Need for validation, traceability, accountability for recognition & promotion & future funding



http://en.wikipedia.org/wiki/File:DirkvdM_natural_spiral.jpg

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Dissemination

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

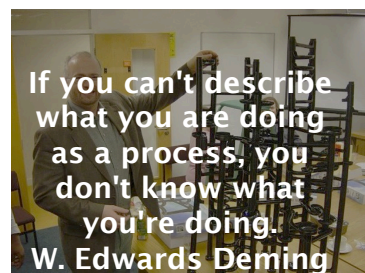
Problems with interdisciplinary research

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How do we communicate?

- Surprisingly difficult to explain what a process involves
- Much of the detail is assumed to be understood and not explicitly discussed
- This is where the miss-understandings usually arise.



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Smart Tea Project

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)

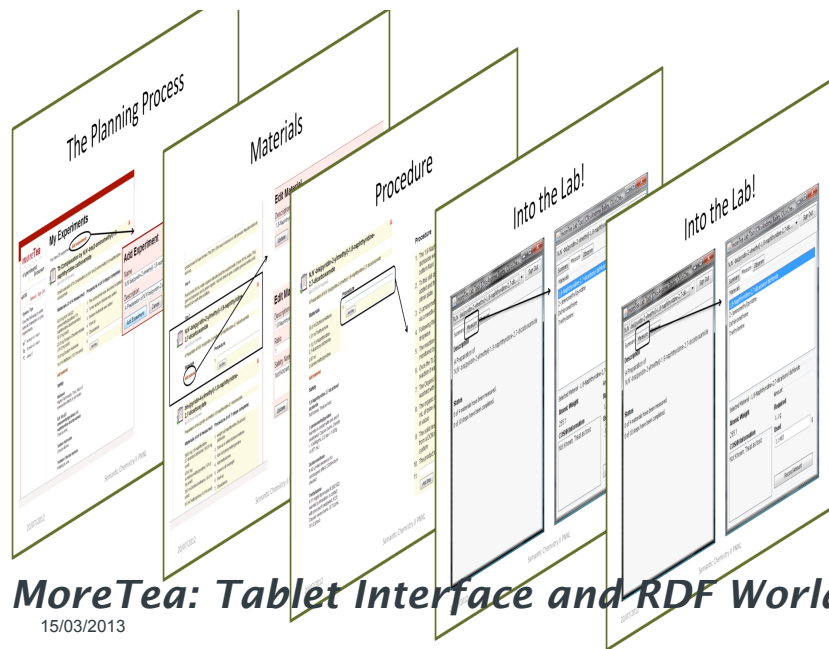
[Guardian story \(and abbreviated version\)](#) of this BSI prize winning document.

[Counterfeit tea \(or smouch\)](#)
– The BBC (and Michael Quinion for the explanation of smouch)

P2 - Plans & Provenance

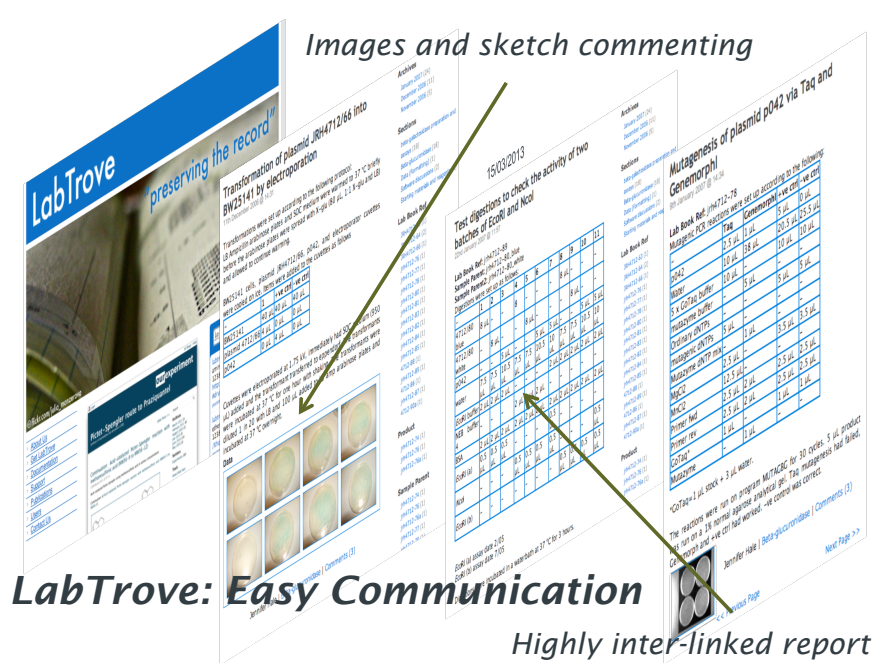
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MoreTea: Tablet Interface and RDF World

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LabTrove: Easy Communication

Highly inter-linked report

Top Methyl ester Hydrolysis- Method 2

9th April 2009 16:50

Lab Note Book Or Experiment Code: FDH-5405-E7P26

Post Type: Method_2

Procedural Step: Method_2

Date Of Experiment: 27-11-08

Experiment Name: Top Methyl ester Hydrolysis

Experiment Code: FDH5405-E7P26

Date of Experiment: 27/11/08

- reaction mixture added to 100ml of DCM
- solid formed... dissolved in DCM/MeOH + water and evaporated to near dryness
- re dissolved in 200ml chloroform + 20ml MeOH, sonicated most degassed
- 30ml water added mydells leading to solid problems and no separation seen.
- 100ml water added now gives clear layer with mydells below
- transferred to bigger 500ml sep funnel

this picture taken directly after transference

- approx. 30ml 2M hydrochloric added to give emitate separation, and turn porphyrin protonated green.
- much better behaved now...lovely shade of green too.

protonated porphyrin with 2M HCL

- HCL reextracted with 100ml CHCl3.
- fluffy brown noted between interface, contaminant?
- organic rinsed 5 times 100ml water. first rinc turns it back to puple

now purple organic with aqueous

- water re-extracted into chloroform 100ml and rinse 5 times h2o.
- organic fractions combined and dried over anhydrous sodium sulfate

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

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

1,4-Benzoquinone (1)
5,6-Methyl Benzene
10,15-Bis-2,4,6-Triethyl Porphyrin

Diversity and Disability

Room Blogs

Laser Environment

46:1047 - 2009-7-20

46:1047 - 2009-7-17

Chamber (46:1047) hysp(thermocouple)

Plant Room (46:1047) hysp(thermocouple)

Shelf top (46:1047) hysp(thermocouple)

Laser box (46:1047) hysp(thermocouple)

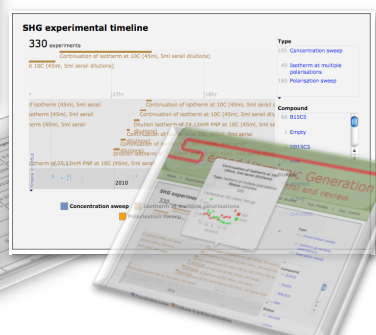
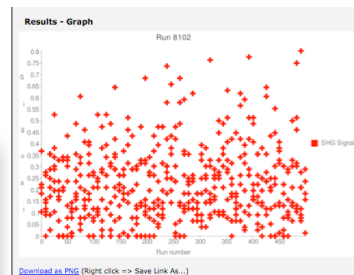
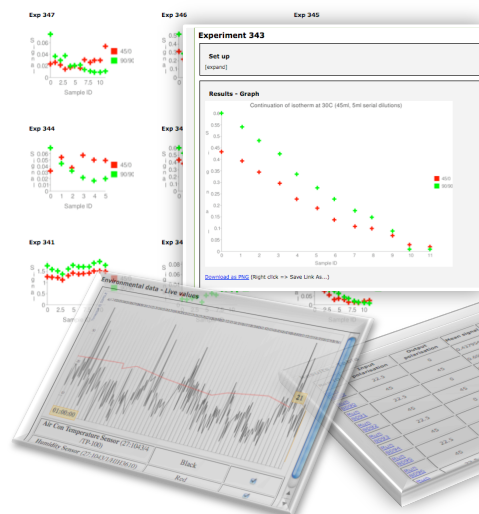
Physical and Digital Worlds

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Second Harmonic Generation Experimental control and review

Liquid interface experiments



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

Title*

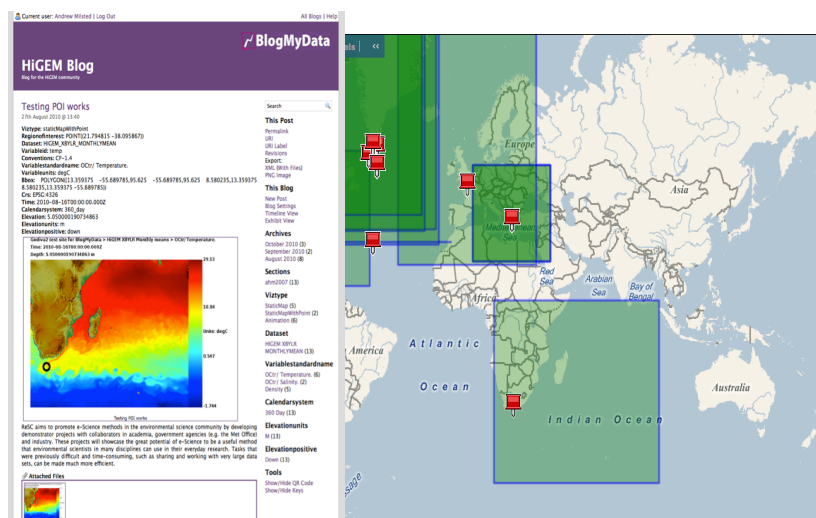
Re: TLT660/4b Hot Stage Video

Text*

QR Code

Digital and
Physical

BlogMyData Project - Godiva



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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 of presentations/reports
- Change the nature of Professor/Student interactions

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

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Sample Originator: Michael B. Hursthouse, Simon J. G. Cox, David R. Taylor, Robert M. Waymouth, Peter D. Tucker, G. McKimming and Mark E. Light.

C₄₄H₅₀N₂O₆

InChI=1/C22H25NO3/c1-23(11-13-25-16-15-24-2)/h3-10,17H,2-11,19H

Identification Number: 10.3737/ecr-2014-26-20-9-5-3-7-1

Date Created: 17 January 2014

Deposited On: 21 Jan 2014

Deposited By: A.N. Admin

(If you need more space to type, click the "Toggle full screen mode" icon)

Advanced

Tags

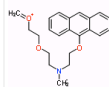
Crown, Crystallography

Category

eCrystals

New Category

Save Changes or Cancel

ChemSpider ID	InChI Key	Basic Info
 21389224	XUOPMAWJUNALK-UHFFFAOYAO InChI=1/C22H25NO3/c1-2	2-[2-{[2-(9-anthryloxy)ethyl]-methanidylamino}ethoxyethyl]-methylene-oxygenium Molecular Formula: C ₂₂ H ₂₅ NO ₃ Molecular Weight: 351.439 Nominal Mass: 351 Da Average Mass: 351.439 Da Monoisotopic Mass: 351.183 Da

04/07/2012

Unilever e-Science

***Making use of
publicly
available
Chemistry Services***

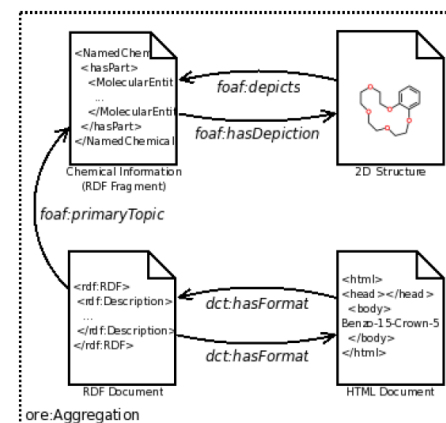
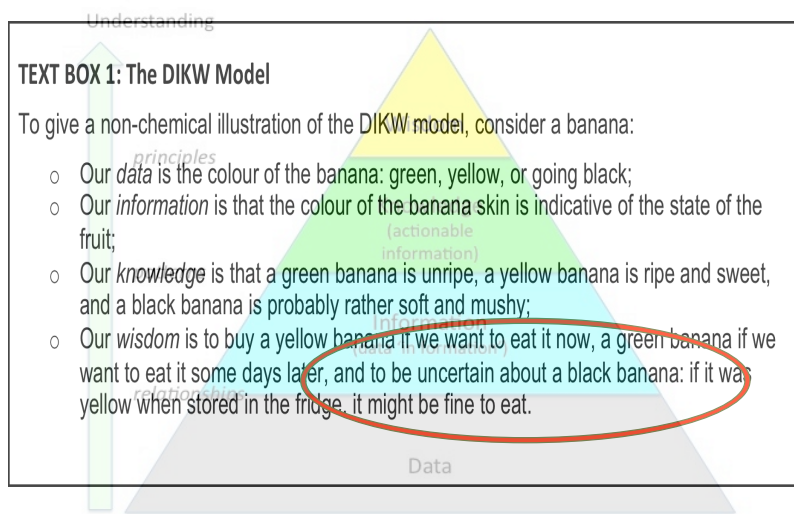


FIGURE 3.18: Depiction of OAI-ORE aggregation of information resources associated with an RSC ChemSpider record.



Uncertainty

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”

Search: ELabtrove

Public Blog Post: Synthesis of 1-amino-2-methyl-1-oxopropan-2-yl 1-(4-fluorophenyl)-2,5-dimethyl-1H-imidazo[3,2-d]pyrimidin-6-yl benzenesulfonamide... [#malaria #drugdesign](http://t.co/GnTcN09l)

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

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

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

Ronakelly13, [-] Thu 16 Aug 11:27 via Paper.li

Public Blog Post: Synthesis of 3-(4-(2-amino-2-methyl-1-oxopropan-2-yl)benzenesulfonamido)-2,5-dimethyl-1H-imidazo[3,2-d]pyrimidin-6-yl benzenesulfonamide... [#malaria #drugdesign](http://t.co/yPelaSUX)

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

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

Public Blog Post: Synthesis of 3-(4-(2-amino-2-methyl-1-oxopropan-2-yl)benzenesulfonamido)-2,5-dimethyl-1H-imidazo[3,2-d]pyrimidin-6-yl benzenesulfonamide... <http://t.co/UNtoGQSV> Top stories today via @BiblioBuster @labtrove @a100ciacerta

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LabTrove Open Notebooks Mat Todd's PZQ Project

PZQ

Praziquantel – Open Science

our experiment

Pictet-Spengler route to PZQ

KAB17-1 (N-benzoyl PZQ analogue). Peptide Acetal KAB17-1 373.1 mg (0.936 mmol), toluene: 39 mL, TiOH: 4.32 µL, 37 mL, TiOH: 4.14 µL (0.047 mmol, 5 mol%).

KAB17-2 (PZQ). Peptide Acetal KAB17-2 394.2 mg (0.974 mmol), toluene: 39 mL, TiOH: 4.32 µL, 37 mL, TiOH: 4.14 µL (0.047 mmol, 5 mol%).

Reaction progress by TLC

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, 5:5, v/v and stained with KMnO₄.

Racemic Resolution of Praziquantel

Hydrolysis of PZQ

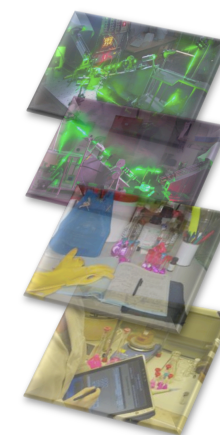
Introduction

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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

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Blog Syn

Crowdsourcing meets Organic Synthesis. Speed and Aplomb.

Blog Archive

▼ 2013 (5)

► March (1)

▼ February (2)

Blog Syn
#003:
Benzylic
Oxidation of
Acylindane
s ...

Blog Syn
#002:
Pd-Catalyze
d C-3
Selective
C-H Olef...

► January (2)

Tuesday, February 12, 2013

Blog Syn #002: Pyridines

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

Updated: 2/20/13 - Adde

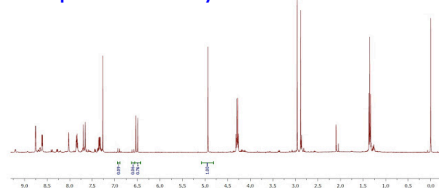
Ref: Yu, M.; Gao, G.-L.;
Experimenters: Two - St

Recommendation: Pendi
Initial - Moderately repr
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 (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?

-SAO

© Cartoonbank.com



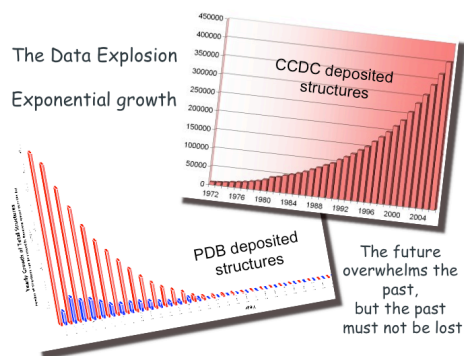
"We have lots of information technology. We just don't have any information."

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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?



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Peony



<http://en.wikipedia.org/wiki/File:PaeoniaSuffruticosa7.jpg>

P&E

"An ontology for Planning and Enactment"

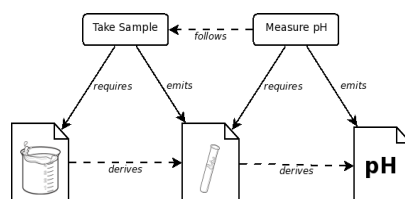
"In theory, there is no difference between theory and practice. But, in practice, there is."

Unknown (possibly Yogi Berra)

15/03/2013

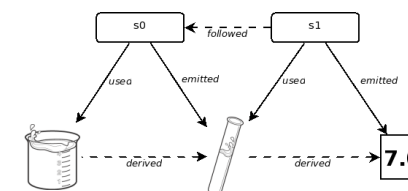
P&E Ontology: Planning

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



P&E Core Ontology: Enactment

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



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Southampton University

eCrystals

Home | About | Browse by Year | Browse by People

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 and Michael B. Hursthouse^a

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

University of Southampton

Chemical Formula: C₁₄H₁₂O₅

Identificat Numb: 14H1-4H1.5

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

Creator: W. Hursthouse

Date: 2005

Stages (10)

Stage: 1 plan.pdf

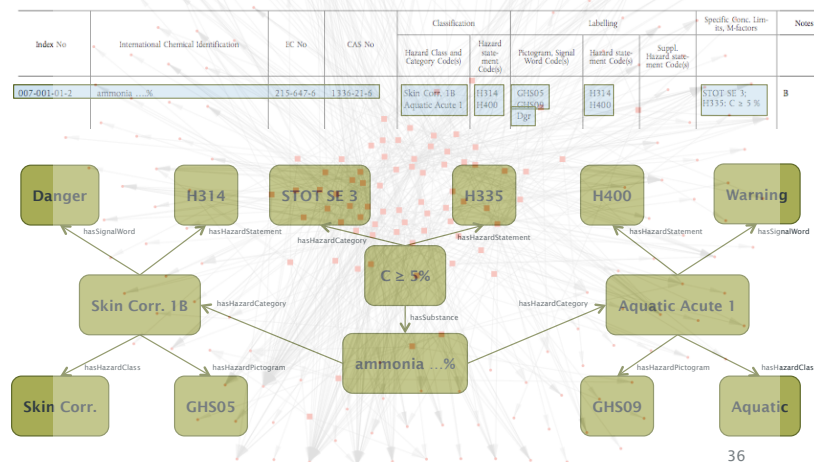
2 plan.pdf

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Chemical Structure Diagram

Example: "ammonia ...%"



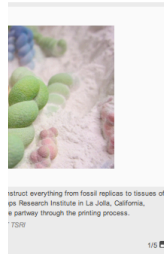
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Change in the whole way we design and build



Digital fabrication is so much more than 3D printing

By Olivia Solon | 13 March 13



It's not everything from fossil replicas to tissues of the Research Institute in La Jolla, California, is partway through the printing process.

1/5

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



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POLITICS HEALTH ECONOMY ENVIRONMENT CULTURE EDUCATION MAGAZINE

Chemist and Pope: Quite a Formula

March 13, 2013 • By Tom Jacobs • No Comments and 48 Reactions

The new pope, Argentinian Jorge Mario Bergoglio, is a startling choice for a [number of reasons](#). He's the first pope from South America, the first Jesuit, the first to take the name Francis.

Lost in all the excitement is the fact that, in all probability, he's also the first [chemist](#) to head the Roman Catholic Church.

A few days ago, we noted the lack of science, as well as social-science, degrees on the part of the current crop of Catholic cardinals. So we'd be sinfully remiss to ignore the fact that Bergoglio defies that trend.

The New York Times reports:

He came relatively late to the priesthood, enrolling in a seminary only at the age of 21, after earning a degree in chemistry.

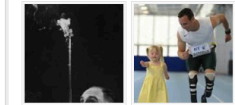
By all accounts, he was a brilliant student who relished the study not just of theology but also of secular subjects such as psychology and literature.

Sounds like a man of wide-ranging intellectual curiosity. There's something gratifying about the notion of a pontiff who could, if needed, analyze the properties of the white smoke that signified his election.

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Is Islam 'Worse' Than Any Other Religion?

For Dying Cancer Patients, Georagov is

ITaaU Network

IT as a Utility

funded under Research Council UK's Digital Economy theme

The Digital Economy vision is of the transformational impact of digital technologies on all aspects of life.

What are we?

IT as a Utility (ITaaU) is one of the 4 sub-themes of the RCUK Digital Economy programme. The ITaaU Network purpose is to promote and enhance the community interested in this aspect of the DE programme and help co-ordinate activities in this area.



First two successful pilot projects recently confirmed:

- **Trusted Tiny Things** – led from University of Aberdeen
- **Using Wireless Networks to Support First Responders and Resilience in Upland Areas** – led from QMUL & Cambridge

Pilot projects

Over the next 3 years we will periodically issue calls for Pilot Projects in the ITaaU area. These will be projects of up to £50k.

The first two successful pilot projects have just been launched.



Call 1 now open

“a temporary transfer to a new research environment”

Secondments

Over the next 3 years we will periodically issue calls for Secondment Projects in the ITaaU area between academic and industrial, commercial or governmental research groups.

opportunities for career development, sectoral knowledge transfer and access to short term skills for project development

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

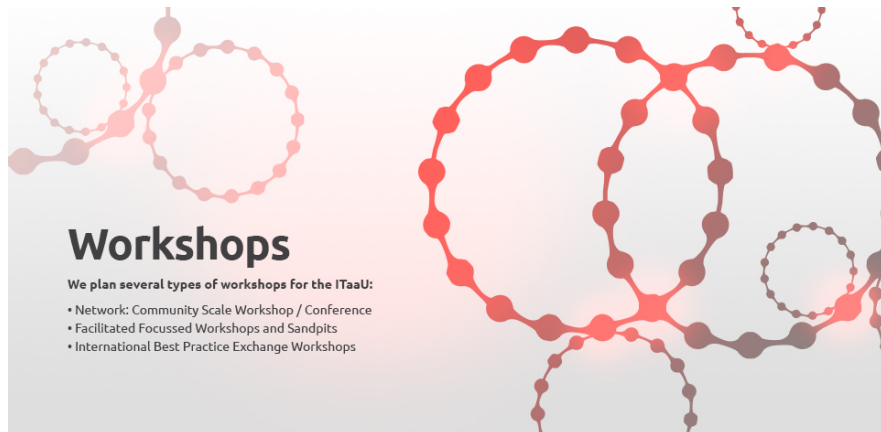
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- Smart Spaces and Diversity
- Emerging Economies: International Perspectives
- Libraries of the Future
- Broadcast Media and Social Media
- Data as a Utility, Hardware as a Utility
- Plus:
- Sandpits and Workshop+ events
- International Best Practice Exchanges

Workshops

We plan several types of workshops for the ITaaU:

- Network: Community Scale Workshop / Conference
- Facilitated Focussed Workshops and Sandpits
- International Best Practice Exchange Workshops



UK must bridge 'valley of death' stopping research being commercialised

By Olivia Solon | 14 March 13



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



15/03/2013

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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

"Trust me Mort
vast and sophisticated"

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