Title: Science in the open /or/ How I learned to stop worrying and love my blog

Date: Sep 12, 2008 11:00 AM

URL: http://pirsa.org/08090038

Abstract: The idea behind the \'Open Science Movement\' is that by making data, results, and protocols freely available to the research community for use and re-use a step change in the efficiency of carrying out science can be achieved. In this talk I will discuss the experience of my research group in pursuing \'Open Notebook Science\' in which we make our laboratory notebooks freely available on the web as experiments are recorded. This involves both the development and use of new tools to make the recording process practical and useful and the cultural challenges of convincing other scientists that this is a worthwhile, and not completely foolhardy, approach.

Science in the open

or
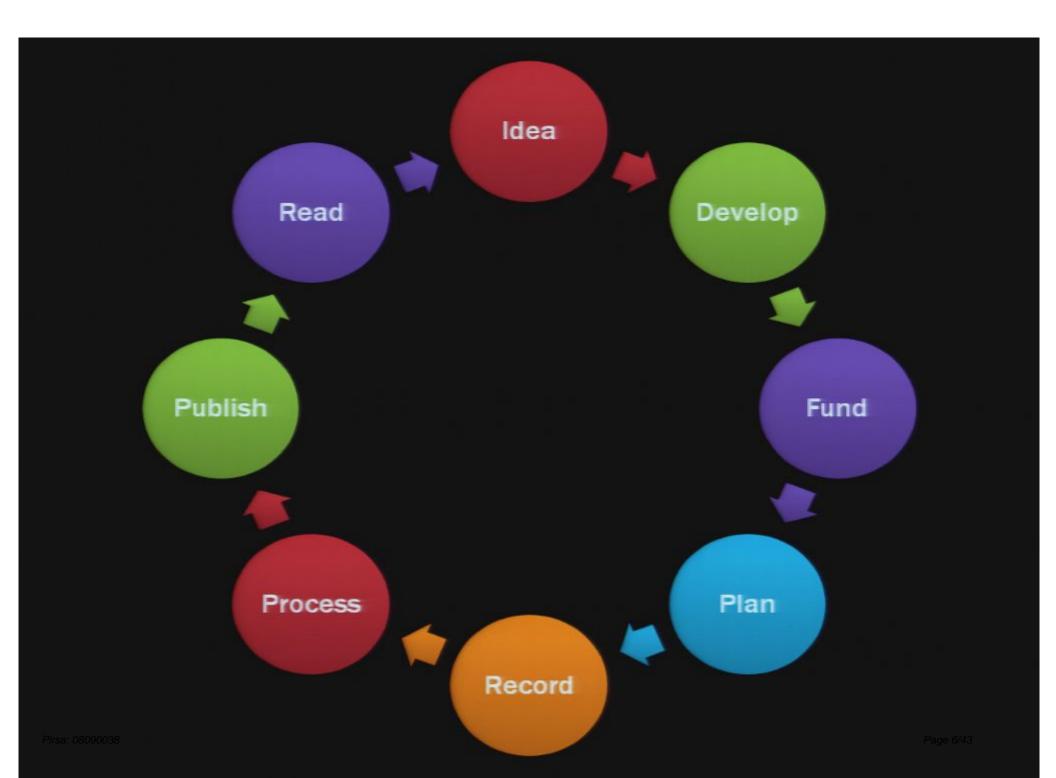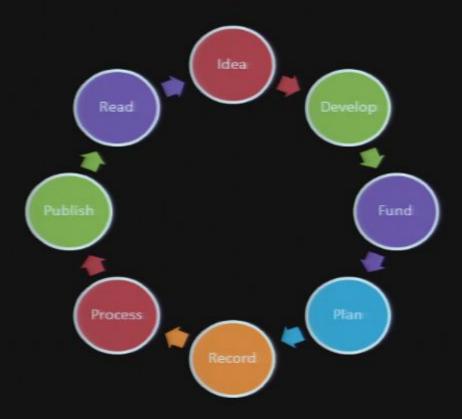
How I learned to stop worrying and love my blog

Cameron Neylon

(with inspiration from many others)

http://www.slideshare.net/CameronNeylon

Some made up numbers...

http://flickr.com/photos/luismimunoznajar/2093185804/
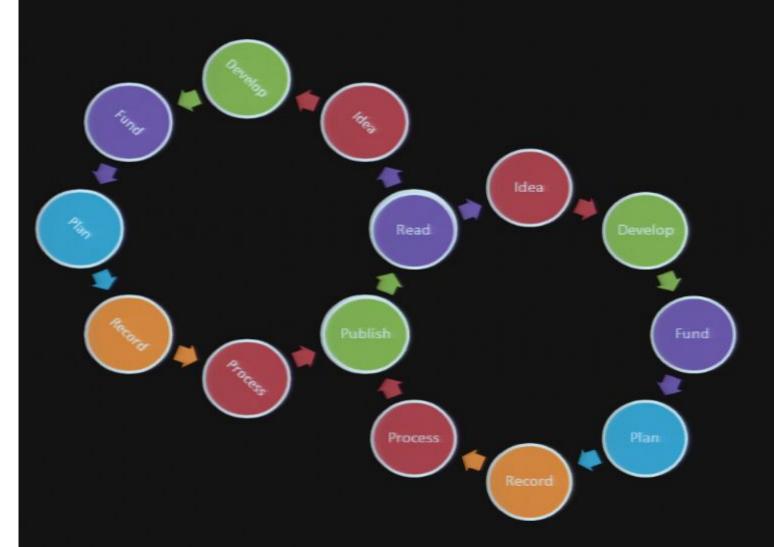
Return on investment...?

http://flickr.com/photos/wwworks/1352842996/
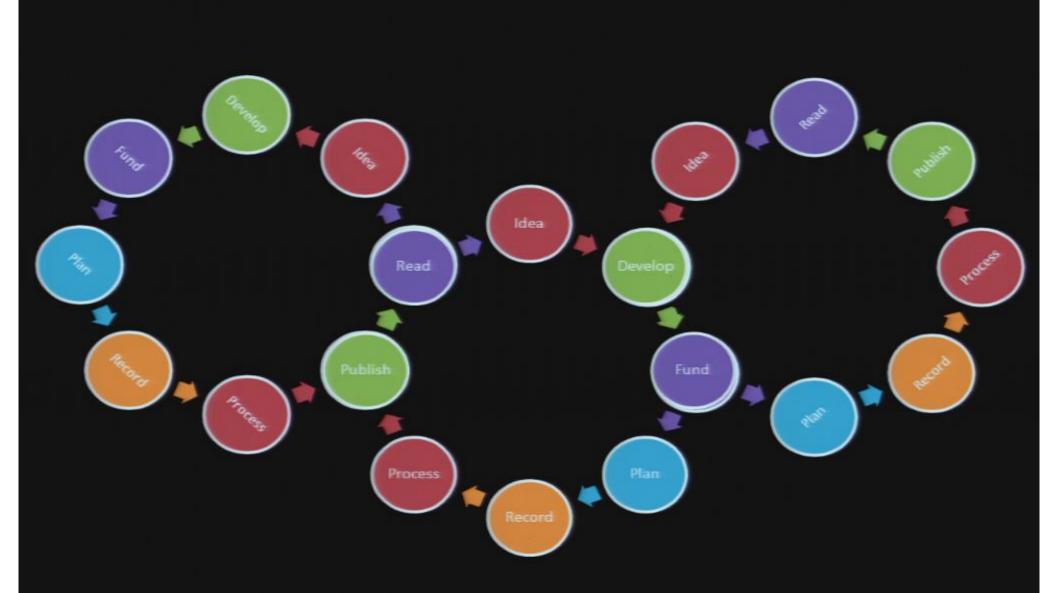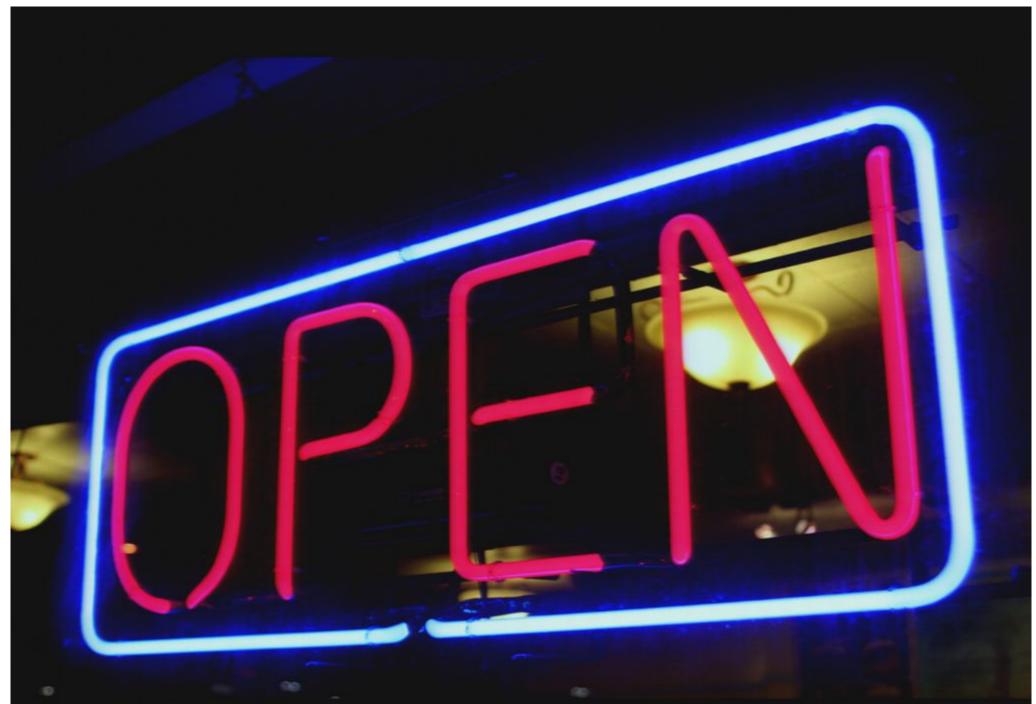
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Sortase Cloning

Weighing of dried samples

4th September 2008 @ 09:05

Instrument: Mettler_4_place_balance
Project: usefulchem_solubility
Post Type: Weighing
The following samples were weighed on a balance tared to zero with a holder in place. i.e. the weight reported is the weight of the sample and the container or tube it is held in.

Sample	Recorded weight (g)
Dried solution of boc-Gly in methanol	1.2063
Dried solution of gly-Ome from methanol	1.0730
Dried solution of vanillin from methanol	1.0799
Dried solution of glucose from methanol	1.0535
Dried solution of mannitol from methanol	1.0534
Dried solution of NaCl from methanol	1.0513
Dried solution of boc-Gly from ethanol	1.1757
Dried solution of gly-OMe from ethanol	1.0546
Dried solution of vanillin from ethanol	1.1232
Dried solution of glucose from ethanol	1.0532
Dried solution of mannitol from ethanol	1.0491
Dried solution of NaCl from ethanol	1.0597
Dried solution of boc-Gly from THF	1.1722
Dried solution of gly-Ome from THF	1.0547
Dried solution of vanillin from THF	1.1673
Dried solution of glucose from THF	1.0500
Dried solution of mannitol from THF	1.0492
Dried solution of NaCl in THF	1.0530

David Neylon | Edit Post | Procedure | Comments (2)

Weighing of empty tubes

4th September 2008 @ 09:57

Done

http://chemtools.chem.soton.ac.uk/projects/blog/blog/blogs.php/blog_id/10

Google

solubility of boc-Glycine in thf   [Search]   Advanced Search
Preferences

Search: ⦿ the web ○ pages from the UK

Web

Near-infrared determination of moisture, fat and protein in Tuna ...
1 Nov 2005 .... Fig 2: 1H NMR of **Boc-glycine**-L-phenylalanine ethyl ester .... However, when
the reaction was carried out in **THF** (to higher **solubility** of the ...
www.usc.es/congresos/ecsoc/9/GOS/a031/index.htm - 143k -
Cached - Similar pages - Note this

[PDF] Template for Electronic Submission of Organic Letters
File Format: PDF/Adobe Acrobat - View as HTML
with N-**BOC-glycine**, followed by deprotection with TFA. Purification of the coupling reaction
..... with anhydrous hydrazine in **THF** to release the desired O- ...
organicdivision.org/essays_2002/hamed.pdf - Similar pages - Note this

UsefulChem » All Reactions
Exp204 Determination of **solubility** of Ugi adduct (99C) in Methanol, Ethanol, Acetonitrile,
Tetrahydrofuran, Acetone, Hexane, Chloroform, and Distilled Water ...
usefulchem.wikispaces.com/All+Reactions - 142k - Cached - Similar pages - Note this

Journal of Fluorine Chemistry : Synthesis of γ-fluoro-α-amino ...
First trials to rearrange the fluorinated **Boc-glycine** esters 4 applying lithium .... However,
change of the solvent from **THF** to the less coordinating diethyl ...
linkinghub.elsevier.com/retrieve/pii/S0022113904004002 - Similar pages - Note this
by F Tranel - 2005 - Related articles - All 2 versions

Imidazolidine antipsychotic agents - US Patent 5332738
tert-butyloxycarbonylglycine (**BOC-glycine**) and dicyclohexylcarbodiimide (DCC)in the
presence of 1-hydroxybenzotriazole with **THF** as solvent, ...
www.patentstorm.us/patents/5332738/description.html - Similar pages - Note this

PROTEIN KINASE C INHIBITORS - Patent EP0766682
The preferred base when the **solubility** of the substrate is not important is ... To the red
solution was added (N- t **BOC)glycine**, p-nitrophenyl ester (0.22 g ...
www.freepatentsonline.com/EP0766682.html - Similar pages - Note this
by JR Gillig - 2001 - Cited by 3 - Related articles - All 12 versions

Recent advances in synthetic micro reaction technology
oxy)silane 9 (1.00 M) in anhydrous **THF** were introduced into ..... sion of **Boc-glycine** 19 to the
respective methyl ester 22, with ...
www.rsc.org/ej/CC/2007/b609428g.pdf - Similar pages - Note this
by P Watts - 2007 - Cited by 5 - Related articles - All 7 versions

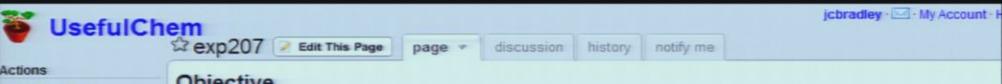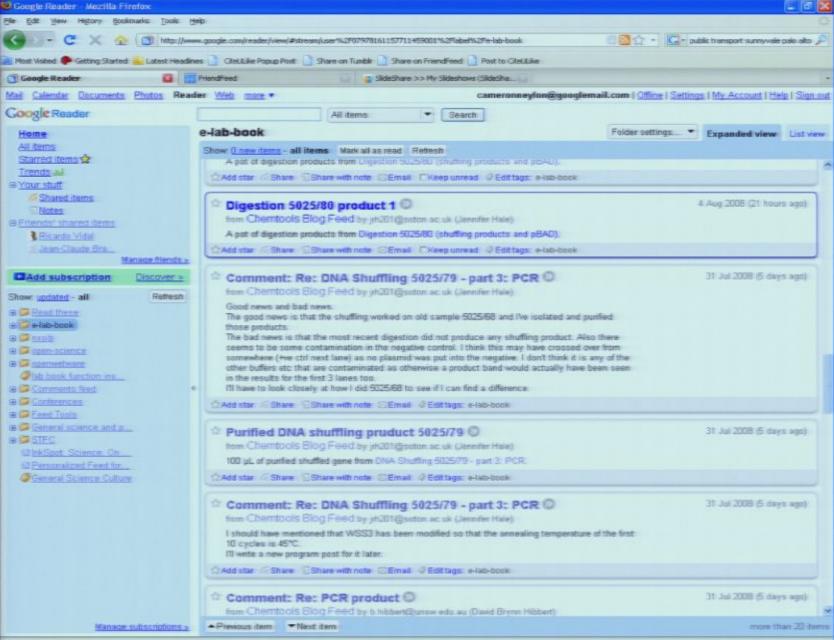Continuous Flow Reactors, a Tool for the Modern Synthetic Chemist
in order to obtain a balance between by-product **solubility** ..... the authors reported quantitative
conversion of **Boc-glycine** 22 to **Boc-glycine** methyl ester ...
doi.wiley.com/10.1002/ejoc.200701041 - Similar pages - Note this

Mechanistic Studies on the Photochemical Deprotection 3',5 ...

9:00 am, 4 September 2008

Southampton Chemistry – 3/9/08

UsefulChem

☆ exp207 ✎ Edit This Page | page ▾ | discussion | history | notify me

Objective

To establish a method of measuring the solubility of some compounds in organic solvents.

Procedure

Solid is added to 1.5 mL Eppendorf tubes containing 500 uL of solvent until saturated after 30 s of vortexing. The tubes are then centrifuged for 60 s then 200 uL of clear solution is transferred to pre-weighed 1.5 mL Eppendorf tubes. The tubes with the clear solution are then evaporated down in a SpeedVac for 2 h and re-weighed to obtain the amount of dissolved solid.

Results

The list of compounds, solvents and measurements is on workbook 207-WB1 🔗
The pics are tagged as EXP207 on Flickr 🔗.

Discussion

This technique was adequate to measure solubilities of the following compounds:
boc-glycine in methanol (4.40 M) and THF (3.45 M)
glycine methyl ester in methanol (1.32 M)
vanillin in methanol (4.19 M) ethanol (2.50 M) THF (3.89 M)

The solubility of boc-glycine in ethanol was measured at 3.57 M but because it appeared as a gel it should be put back on the speedvac to see if a powder can be obtained.

All other compounds measured to less than 5 mg and should be redone using much more solvent to get an accurate measurement.

http://usefulchem.wikispaces.com/Exp207

7:36 pm, 4 September 2008
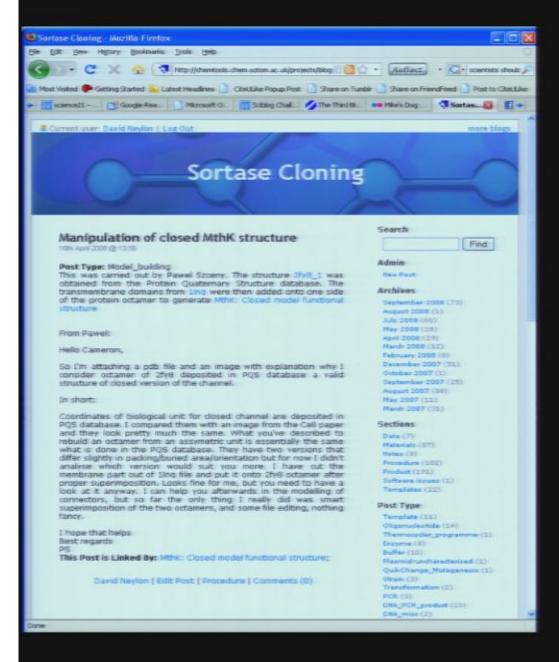
You posted a message
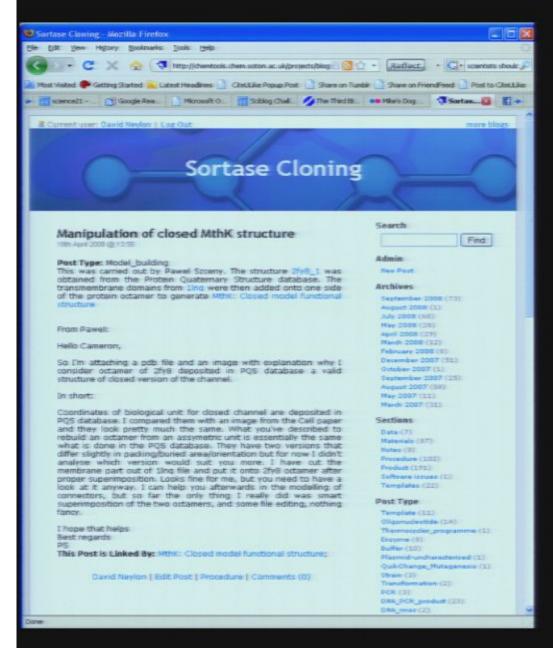
"Request for assistance:"
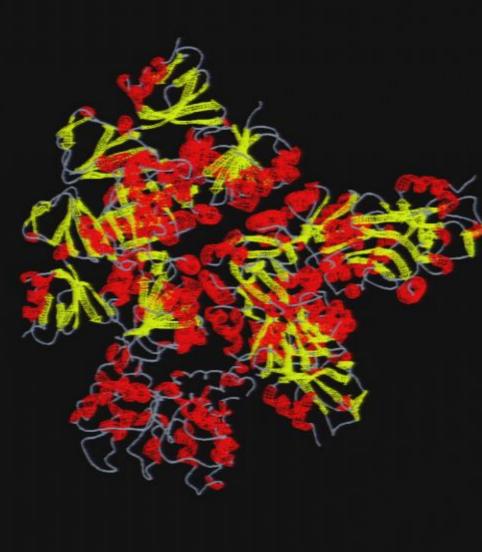
April 11 at 11:53 am - Comment - More ▾

💬 I'm trying to build a model of the calcium gated potassium channel **MthK** using the PDB files 1lnq and 2fy8. **MthK** has a gating domain (rck domain) and a transmembrane domain and works as a tetramer of full length proteins with a tetramer of just rck domain. So I can build the ligand bound (open conformation) from 1lnq by removing residues 19-98 from chains A, B, C, and D. The closed conformation is harder. 2fy8 has the rck domain in the closed conformation but the deposited structure is the asymmetric unit and not the biological unit. What I need to do is build the rck octamer in the closed conformation and then to put that back on top of the transmembrane domain tetramer. Swiss pdb viewer which isn't really cutting the mustard. If anyone can help us by building the models that would be brilliant. Our aim is to determine the structure of these molecules in solution (with detergent) by small angle scattering so good models to compare with data are crucial. Authorship on papers a given - can't offer any money - You (edit | delete)

💬 How fast that needs to be done? I think I can help, but I can start in the middle of the next week. - Pawel Szczesny
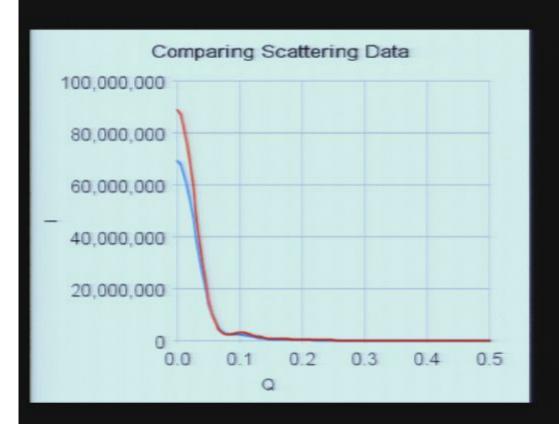
http://friendfeed.com/e/9875b15c-7932-4714-aaba-2a15950219ec/Request-for-assistance/
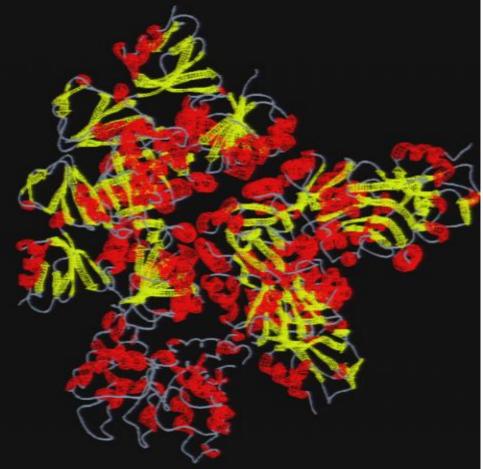http://tinyurl.com/6xj69p

http://chemtools.chem.soton.ac.uk/projects/blog/blogs.php/bit_id/7735

http://chemtools.chem.soton.ac.uk/projects/blog/blogs.php/bit_id/7735

So what are the papers for?

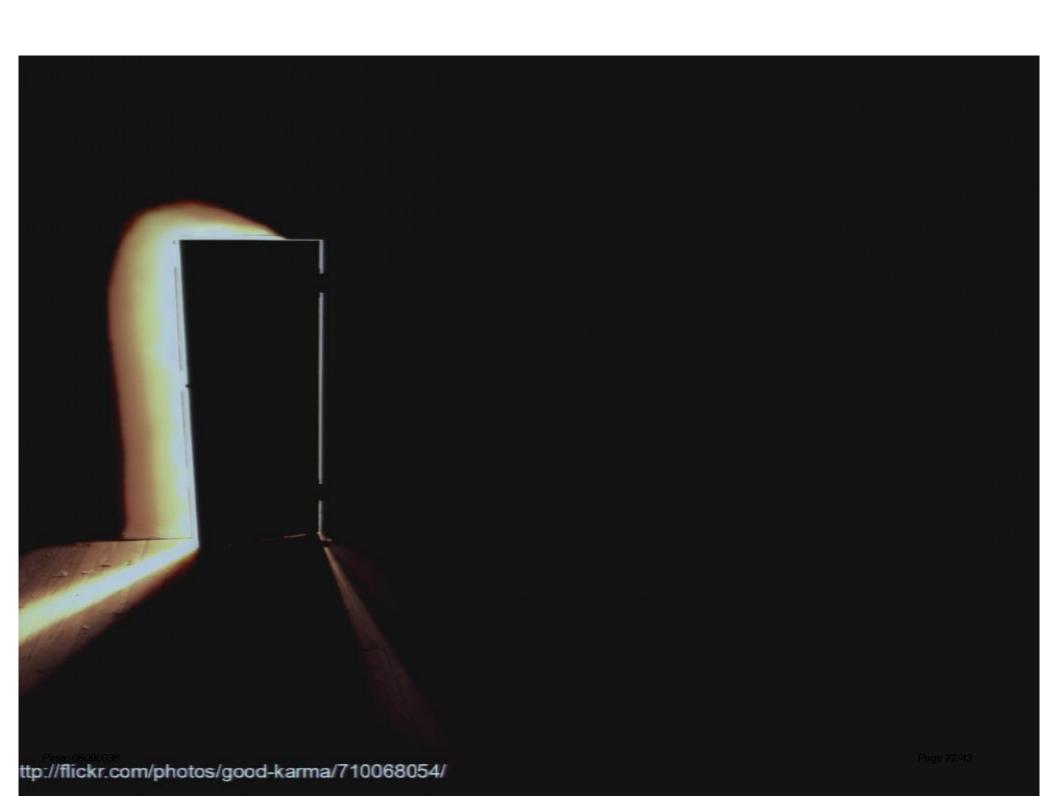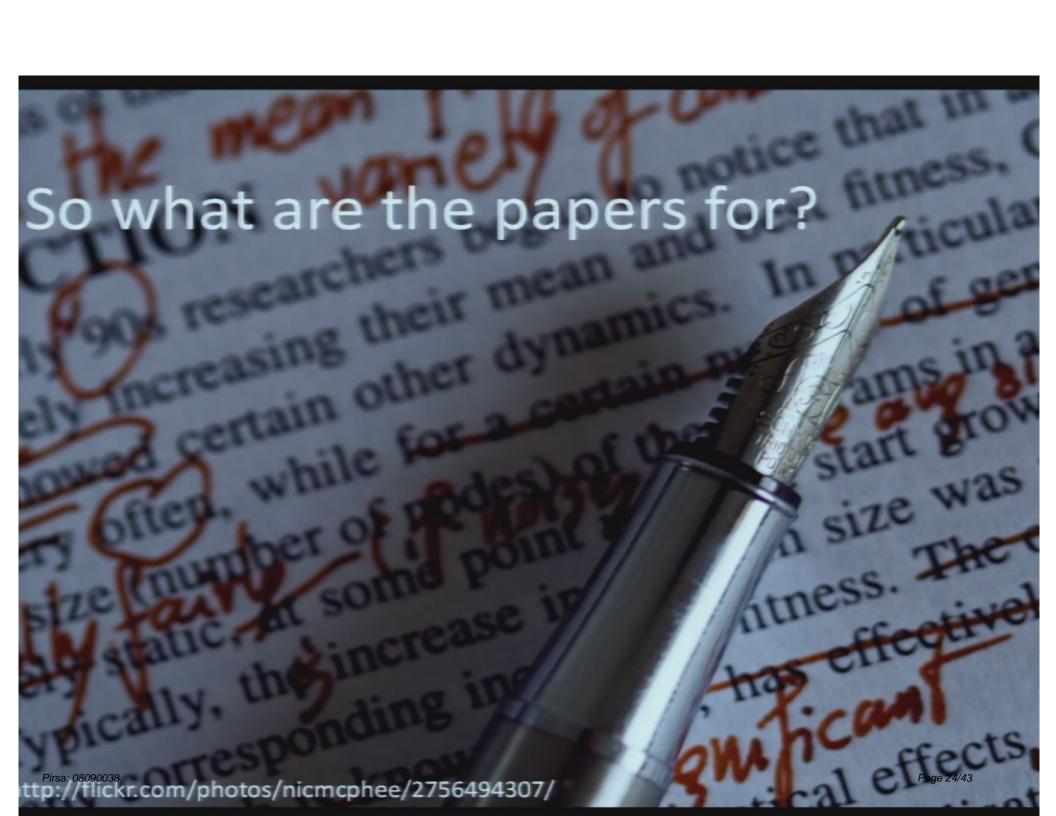http://flickr.com/photos/nicmcphee/2756494307/

A paper = a claim (or claims)
The full record that supports that
claim should be available for
detailed examination and critique

*'We argue in good faith from shared
evidence to shared conclusions'*

Lee Smolin
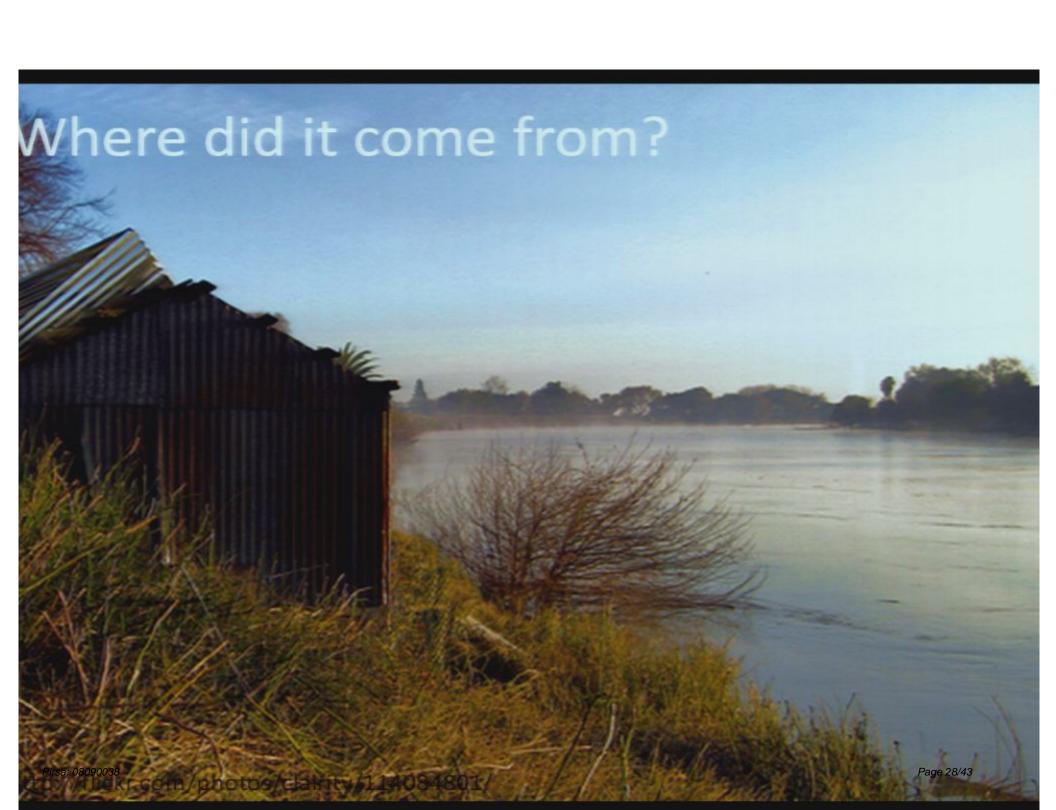
Tools?

Where did it come from?

http://flickr.com/photos/clarity/114084801/

Capture at source

http://flickr.com/photos/jason_burmeister/2053139930/
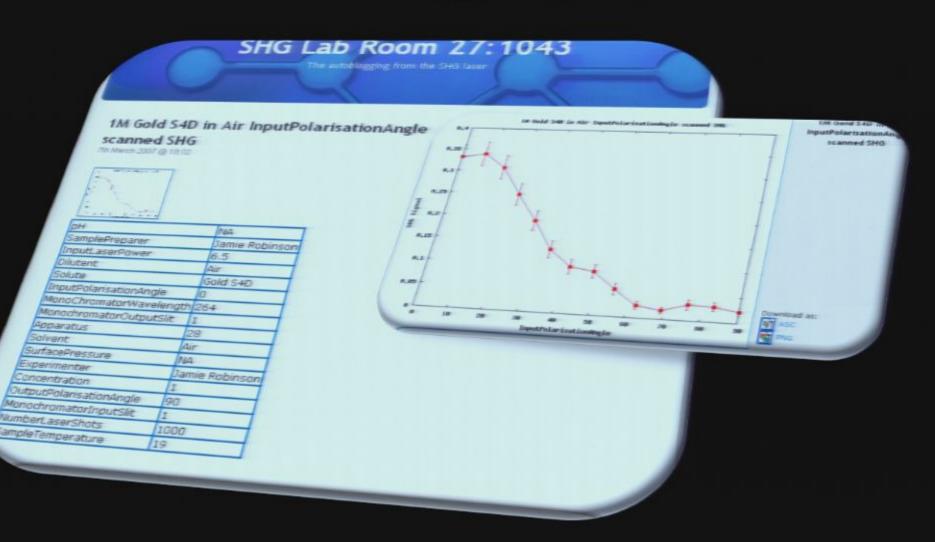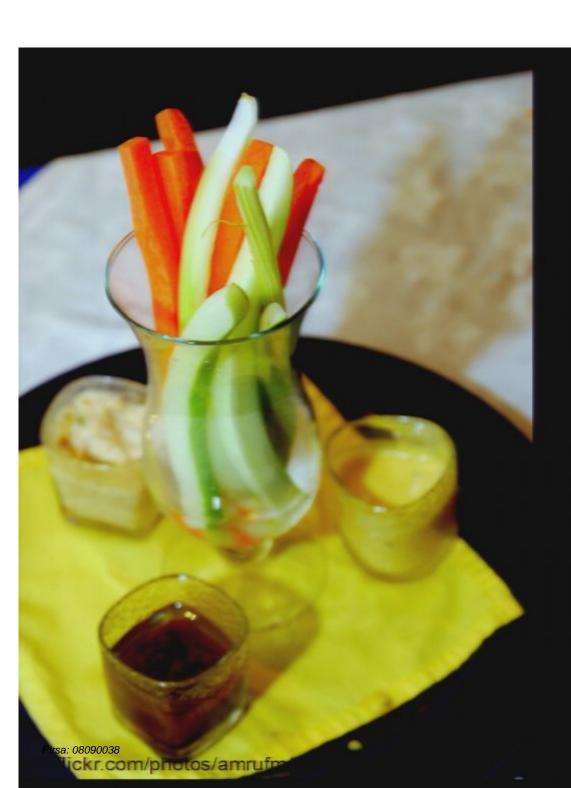
Automatic Blogging by Machines

- Fit the existing workflow

- Outperform

- 100% reliable

- One killer feature

- Prepopulate

1. Fit the existing workflow
2. Compelling *first time* user experience
3. 100% reliable (and able to back up to old system)
4. ≥ One killer feature
5. Prepopulate with available information

Blog Post

ttp://flickr.com/photos/hinkelstone/1357630710/

Policy?

flickr.com/photos/amrufm

The public domain is not an "unlicensed commons". The public domain does not equal the BSD. It is not a licensing option.

It is the natural legal state of data.

John Wilbanks, Creative Commons

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http://network.nature.com/blogs/user/wilbanks/2008/05/10/on-the-erosion-of-the-public-domain
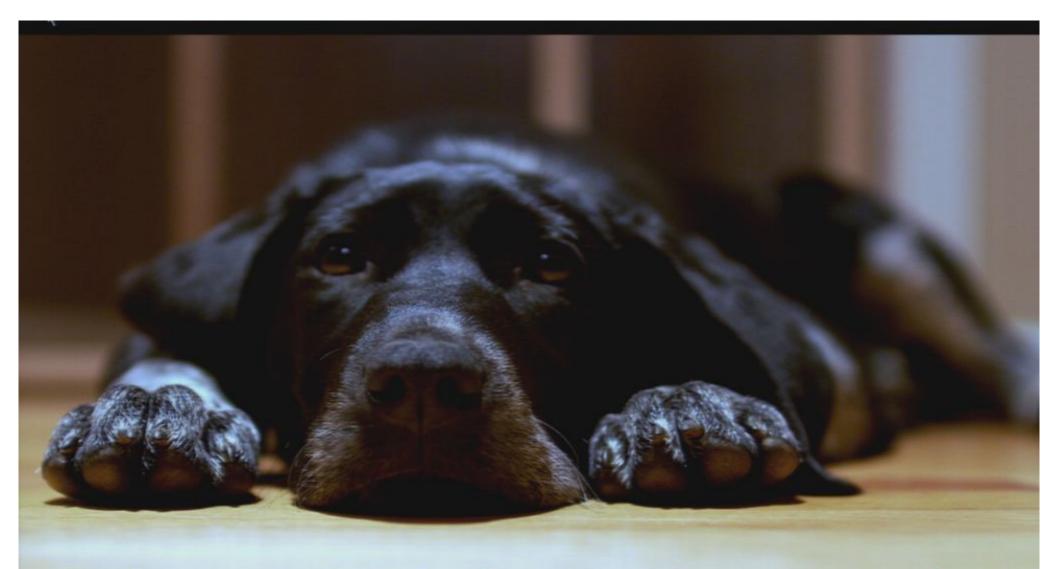
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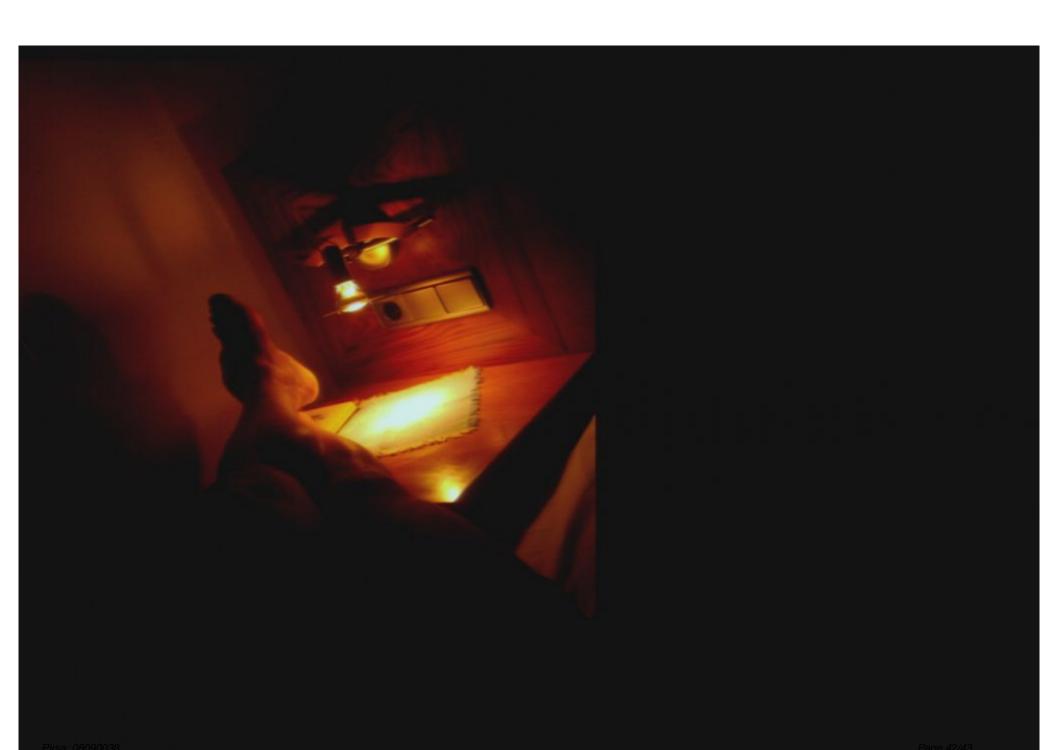http://network.nature.com/blogs/user/wilbanks/2008/05/10/on-the-erosion-of-the-public-domain

'..open data is free...as in a puppy'
Anna Gold, Cal Poly

http://flickr.com/photos/lecates/423460439/

Motivation?