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
http://flickr.com/photos/stansich/433484931/
Some made up numbers...
Return on investment...?
### Weighing of dried samples
4th September 2008 @ 09:02

**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.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Recorded weight (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dried solution of boc-Gly in methanol</td>
<td>1.2063</td>
</tr>
<tr>
<td>Dried solution of gly-Ome from methanol</td>
<td>1.0730</td>
</tr>
<tr>
<td>Dried solution of vanillin from methanol</td>
<td>1.0799</td>
</tr>
<tr>
<td>Dried solution of glucose from methanol</td>
<td>1.0935</td>
</tr>
<tr>
<td>Dried solution of mannitol from methanol</td>
<td>1.0534</td>
</tr>
<tr>
<td>Dried solution of NaCl from methanol</td>
<td>1.0519</td>
</tr>
<tr>
<td>Dried solution of boc-Gly from ethanol</td>
<td>1.1757</td>
</tr>
<tr>
<td>Dried solution of gly-Ome from ethanol</td>
<td>1.0546</td>
</tr>
<tr>
<td>Dried solution of vanillin from ethanol</td>
<td>1.1232</td>
</tr>
<tr>
<td>Dried solution of glucose from ethanol</td>
<td>1.0932</td>
</tr>
<tr>
<td>Dried solution of mannitol from ethanol</td>
<td>1.0491</td>
</tr>
<tr>
<td>Dried solution of NaCl from ethanol</td>
<td>1.0977</td>
</tr>
<tr>
<td>Dried solution of boc-Gly from THF</td>
<td>1.1722</td>
</tr>
<tr>
<td>Dried solution of gly-Ome from THF</td>
<td>1.0547</td>
</tr>
<tr>
<td>Dried solution of vanillin from THF</td>
<td>1.1673</td>
</tr>
<tr>
<td>Dried solution of glucose from THF</td>
<td>1.0900</td>
</tr>
<tr>
<td>Dried solution of mannitol from THF</td>
<td>1.0492</td>
</tr>
<tr>
<td>Dried solution of NaCl in THF</td>
<td>1.0530</td>
</tr>
</tbody>
</table>

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

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http://chemtools.chem.soton.ac.uk/projects/blog/blog/blogs.php/blog_id/10
Southampton Chemistry – 3/9/08
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.
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.

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
Sortase Cloning

Manipulation of closed MthK structure
19th April 2009 @ 13:08

Post Type: Model_building
This was carried out by Pawel Szczepan. The structure 3h8T was obtained from the Protein DataBank Structure database. The transmembrane domains from 1kg were then added onto one side of the protein octamer to generate MthK: Closed model functional structure.

From Pawel:

Hello Cameron,

So I'm attaching a pdb file and an image with explanation why I consider octamer of 3h8T deposited in PDB database a valid structure of closed version of the channel.

In short:

Coordinates of biological unit for closed channel are deposited in PDB database. I compared them with an image from the Cell paper and they look pretty much the same. What you've described to rebuild an octamer from an asymmetric unit is essentially the same what is done in the PDB database. There are versions that differ slightly in packing/buried area/orientation but for now I didn't analyse which version would suit you more. I have cut the membrane part out of 3h8T file and put it onto 2h8T octamer after proper superimposition. Looks fine for me, but you need to have a look at it anyway. I can help you afterwards in the modelling of connectors, but so far the only thing I really did was smart superimposition of the two octamers, and some file editing, nothing fancy.

I hope that helps:
Best regards:
Pawel

This Post is Linked By: MthK: Closed model functional structure;

David Neylon | Edit Post | Procedure | Comments (0)

http://chemtools.chem.soton.ac.uk/projects/blog/blogs.php/bit_id/7735
Manipulation of closed MthK structure
18th April 2008 @ 13:58

Post Type: Model building
This was carried out by Pawel Szczyr. The structure 3msh_1 was obtained from the Protein DataBank Structure database. The transmembrane domains from 1mg were then added onto one side of the protein octamer to generate MTM: Closed model functional structure.

From Pawel:

Hello Cameron,

So I'm attaching a pdb file and an image with explanation why I consider octamer of 3msh deposited in PDB database a valid structure of closed channel.

In short:
Coordinates of biological unit for closed channel are deposited in PDB database. I compared them with an image from the Cell paper and they look pretty much the same. What you've described to rebuild an octamer from an asymmetric unit is essentially the same what is done in the PDB database. They have two versions that differ slightly in packing/orientation but for now I didn't analyse which version would suit you more. I have cut the membrane part cut out of 3mg file and put it onto 3msh octamer after proper superimposition. Looks fine for me, but you need to have a look at it anyway. I can help you afterwards in the modelling of connectors, but so far the only thing I really did was smart superimposition of the two octamers, and some file editing, nothing fancy.

I hope that helps:
Best regards
Pawel

This Post is Linked By: MthK: Closed model functional structure:

David Neylon | Edit Post | Procedure | Comments (0)
So what are the papers for?
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
Claim = Analysis + Data + Interpretation
Where did it come from?
Capture at source
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

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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