



Digital & Physical Laboratories

Jeremy Frey
University of Southampton
Champion for IT as a Utility Digital Economy Network



20/07/2012

Semantic Chemistry II PNNL

Talk Outline

The value of the Semantic Web in the laboratory

Jeremy G. Frey
School of Chemistry, University of Southampton, SO17 1BJ UK

The Semantic Web is beginning to impact on the wider chemical and physical sciences, beyond the earlier adopted bio-informatics. While useful in large-scale data driven science with automated processing, these technologies can also help integrate the work of smaller scale laboratories

Review

- Context for our Work
- The LabTrove System
- Tea Time
- Reproducible Future

Expert Opinion
Web-based services for design and discovery
Jeremy G. Frey, School of Chemistry, University of Southampton, SO17 1BJ UK

1. Introduction
2. Web services and workflows
3. Basic components
4. Techniques of drug design and discovery
5. Network services
6. Systems approaches
7. Semantic web techniques for

20/07/2012

Semantic Chemistry II PNNL

UltraFast Xray Group

UNIVERSITY OF Southampton

<< Next Post Previous Post >> Search

Timeline

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

Jun 12 Jun 13 Jun 14 Jun 15 Jun 16 Jun 17 Jun 18 Jun 19 Jun 20 Jun

May Jun Jul Aug

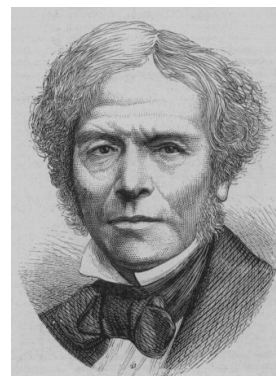
20/07/2012

Semantic Chemistry II PNNL

ON BEING A SCIENTIST

A GUIDE TO RESPONSIBLE CONDUCT IN RESEARCH

THIRD EDITION



20/07/2012

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'

Semantic Chemistry II PNNL

***The academics
media profile!***

- Store of data that can be viewed and manipulated in different ways
- User interfaces to suite user and occasion

He is charged with expressing contempt for meta-data

LabTrove Users

The collage features several overlapping web pages from the University of Southampton:

- Decision Environment for Complex Design Evaluation**: A page with a red and white aircraft graphic and text about a flight test plan for the T-100.
- UNSW eBook**: A page with the text "It's not only what you know, but also how you know it."
- ourExperiment**: A website for sharing and running experiments, featuring a "Project Lab Books" section.
- Engage Lab Book**: A page titled "Engage Lab Book" with a "Share this" button.
- UltraFast Xray Group**: A page with a blue header and a "Measured pump-field output from cavity" section.
- blogs@ChemTools**: Two blog pages with titles like "DECONTAMINATE! Shovelers test 17 September" and "The 2 data sets are 6 x 6, 3D spatial maps of the last two columns as a function of time." They include sections for "Project Blogs", "Bio Blogs", "Engaging Machines", and "Environment Blogs".
- Godiva Blog**: A page with a blue header and a "The 2 data sets are 6 x 6, 3D spatial maps of the last two columns as a function of time" section.
- Division Space**: A page with a blue header and a "Division Space" section.
- Lab Notebooks**: A page with a blue header and a "Lab Notebooks" section.
- Southampton**: A page with a blue header and a "Southampton" section.

The bottom of the collage shows a date stamp "20/07/2012" and a text "Semantic Chemistry II PNL".

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/MuOH + water and evaporated to near dryness
- re dissolved in 200ml chloroform+20ml MeOH, sonicated most dissolved
- 30ml water added myselfs leading to solid problems and phase separation seen.
- 100ml water added now gives clear layer with mixture below
- transferred to bigger 500ml sep funnel

this picture taken directly after transference

- approx. 30ml 2Mhydrochloric added to give emitate separation. and turn porphyrin protonated green.
- much better behavior 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.
- organicfractions combined and dried over anhydrous sodium sulfate

Experiment Name
Preparation Of Porphyrinoids
Alcohol, Phenols And Salts (1)
Preparation Of N-Glycoside
Lactone-Hydrolysis (1)
Solid Acetate (1)
Preparation Of P-tert Butyl
Oxidation (1)
Galla (1)
Preparation Of Mono Para Methyl

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

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	orange	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?/contaminat?
1	6mm	0.21	yes	n/a	orange	n/a	n/a	product.

1,4-Benzoquinone (1)
5,6-Methano Derivative
10,15,20-tri Phenyl Porphyrin

Diversity and Disability

20/07/2012

Semantic Chemistry II PNNL

Impact on researchers

- Higher Quality Record
- Easier Collaboration
- Improved planning
- Improved discussions
- Efficiency gain in production of presentations/reports
- Change the nature of Professor/Student interactions



"Are we thinking here, or is this just so much pointing and clicking?"

© 1995 New Yorker Magazine. All rights reserved.
From The New Yorker Book of Technology Cartoons

20/07/2012

Semantic Chemistry II PNNL

Returning to the Lab

or

How to get people to use the systems

Get the Data there before them!

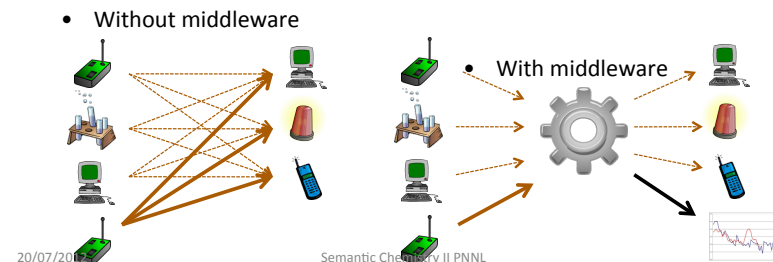
Laboratory Middleware
The SRF LabBroker Software

20/07/2012

Semantic Chemistry II PNNL

Middleware

- Middleware is the connecting software between separated components
- Message brokering system used
- Increases scalability and interoperability



20/07/2012

Semantic Chemistry II PNNL

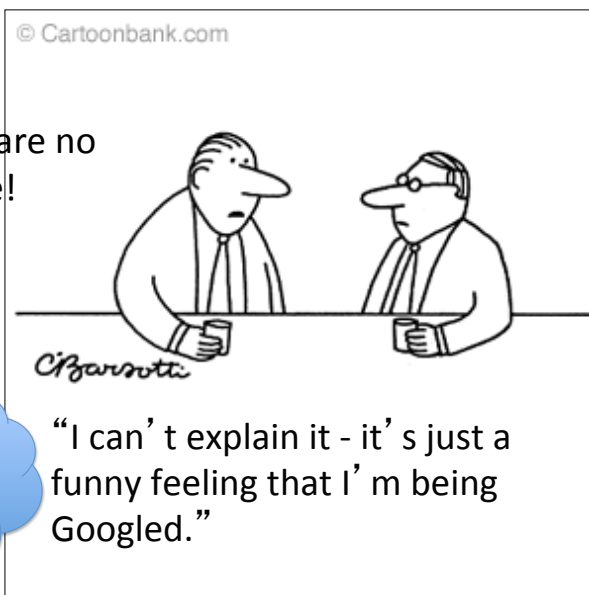
Experimental review



Not just people - Instruments Blog too



People & Data are no different online!



But do you trust the information?

20/07/2012

Semantic Chemistry II PNNL

BBC NEWS

UK version International version About the versions Low graphics Help Contact us

News Front Page World UK England Scotland Wales Business Politics Health Education Science/Nature Technology Entertainment

Have Your Say Magazine In Pictures Week at a Glance Country Profiles In Depth Programmes

Chemists escape labs via mobiles

By Jo Twist
BBC News science and technology reporter

A blend of mobile technology and award-winning software is letting scientists finally escape the lab.

The software, called "middleware", lets different computer systems talk to each other securely and instantaneously.

As part of a national e-Science project in the UK, it is being used to let Southampton University chemists monitor experiment conditions from mobiles.

Sensors in the lab pick up any changes in the environment so the system can alert chemists, wherever they are.

The system is not smart enough to actually buy a round yet

"It replaces the traditional notebook with some electronic form, but it is not just about carrying around a computer - it is much smarter than that," Dr Jeremy Frey, from

SEE ALSO:

- Top UK innovation prize for IBM
- 11 Jun 04 | Technology
- Boom times ahead for smartphones
- 27 Aug 04 | Technology
- E-mail provides Arctic lifeline
- 09 May 04 | Technology
- Heart treatment from a distance
- 11 Aug 04 | Health

RELATED INTERNET LINKS:

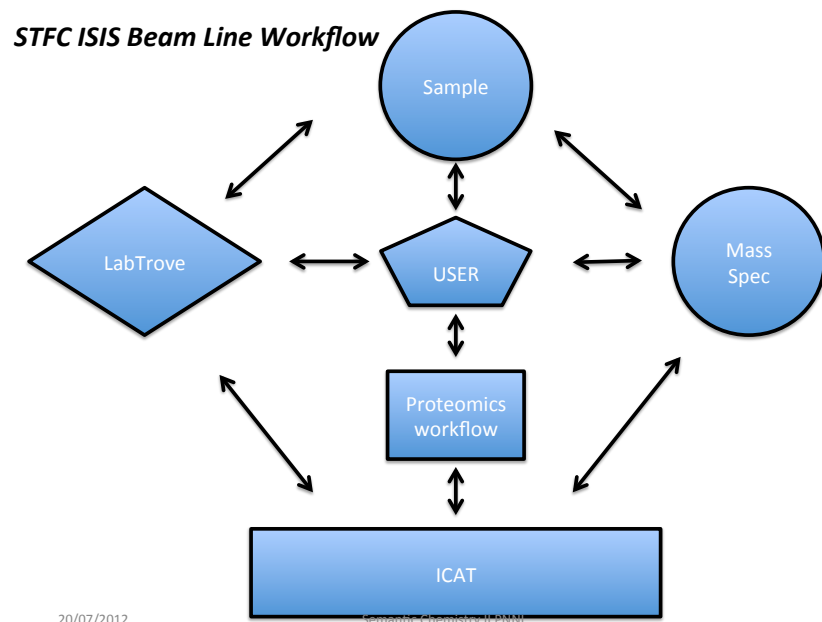
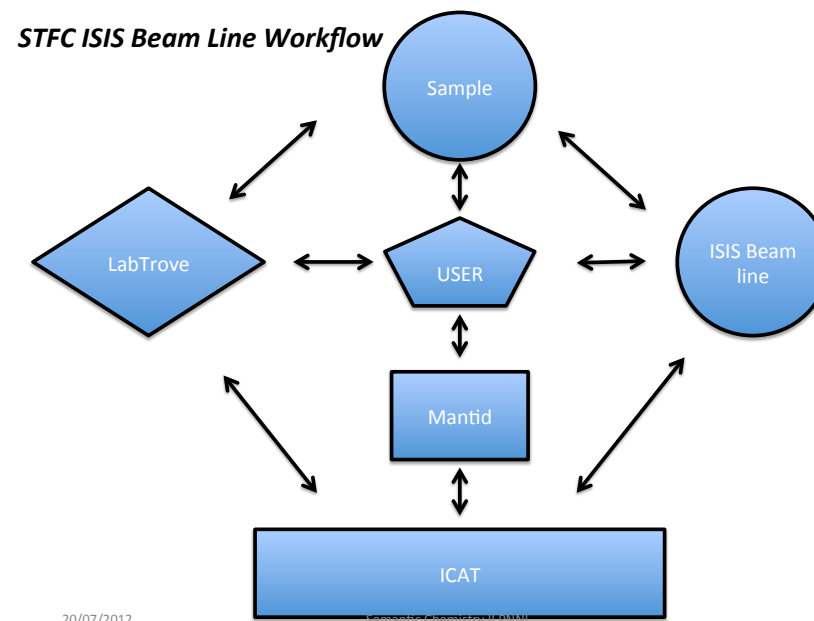
- Dr Frey's group
- University of Southampton
- Combechem (e-Science project)
- IBM Hursely Labs
- EPSC

The BBC is not responsible for the content of external internet sites

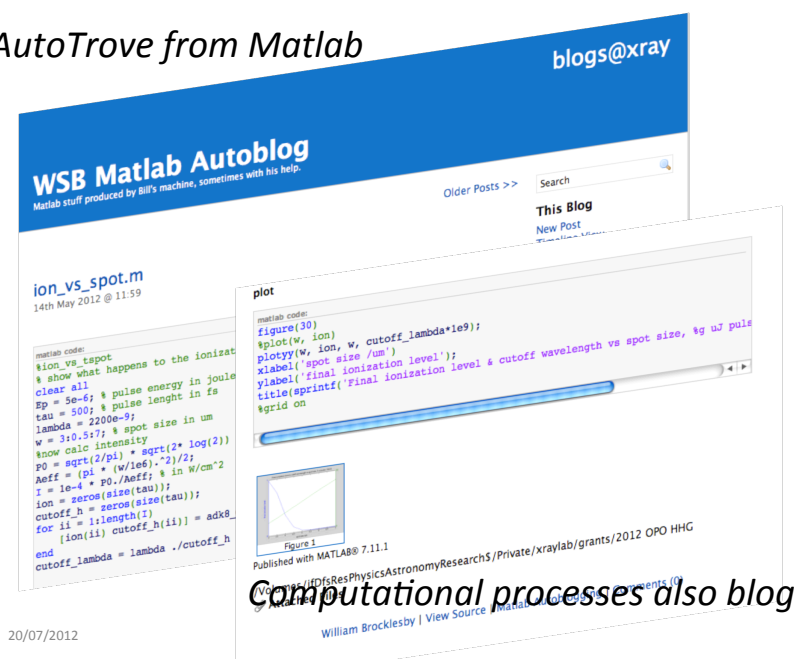
TOP SCIENCE/NATURE STORIES NOW

- 'Pharmed' goats seek drug licence
- DNA 'could predict your surname'
- Bird flu vaccine no 'silver bullet'
- Elephant seals dive for science

RSS | What is RSS?



AutoTrove from Matlab

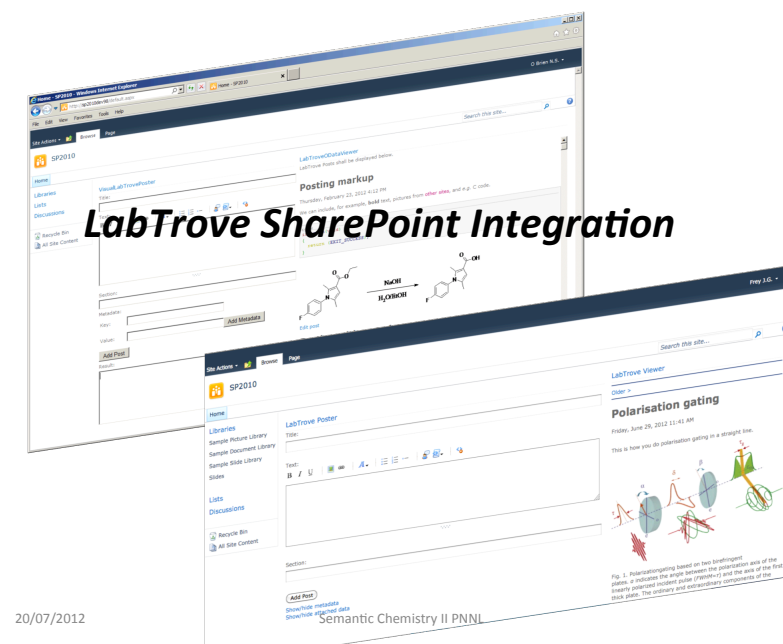




"We have lots of information technology. We just don't have any information."

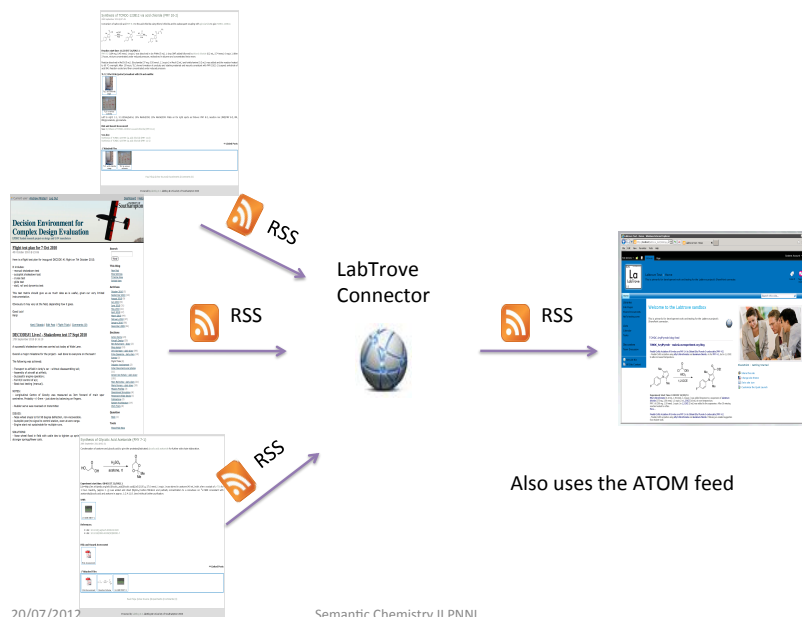
20/07/2012

Semantic Chemistry II PNNL



20/07/2012

OData



20/07/2012

Semantic Chemistry II PNNL

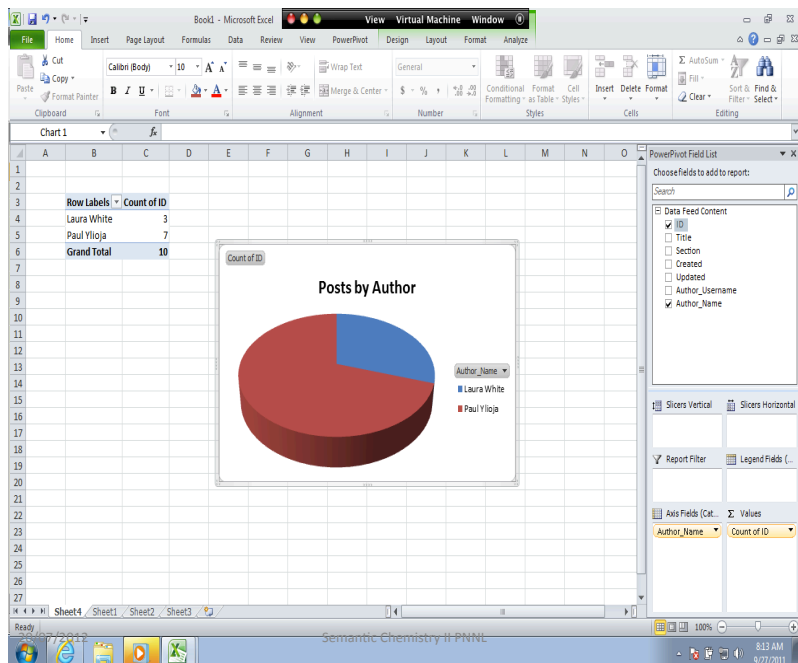
```
<?xml version="1.0" encoding="UTF-8"?>
<service xmlns="http://www.w3.org/2007/app" xmlns:base="http://malaria.ourexperiment.org/odata/tcmcd_ap/" xmlns:app="http://www.w3.org/2005/atom">
  <workspace>
    <atom:title>TCMCD_Arylpyrrole</atom:title>
    <collection href="Posts">
      <atom:title>Posts</atom:title>
    </collection>
  </workspace>
</service>
```

Exampe: http://malaria.ourexperiment.org/odata/tcmcd_ap

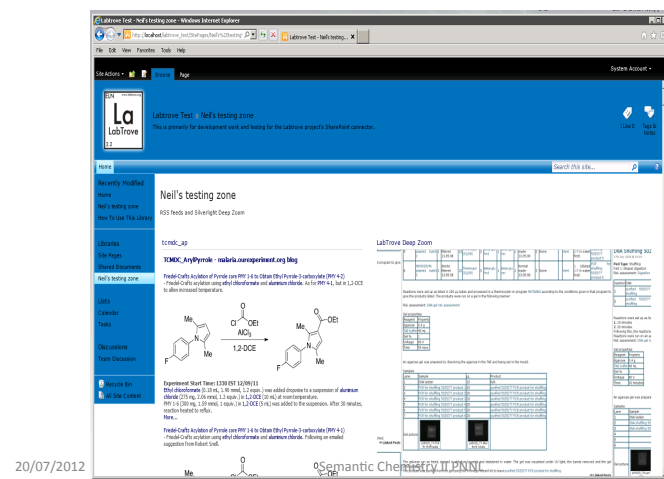
20/07/2012



Semantic Chemistry II PNNL



Adding DeepZoom to SharePoint



If you have a plan then make use of it!

Just like the UK COSHH safety plans are ideal basis for driving an Electronic Laboratory Notebook

With a little extra work a plan becomes a useful way to provide context for the digital record

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 misunderstandings usually arise.



Smart Tea Project

the Smart Tea Project



"I can go anywhere and its, like, this is me and my data. Its all there, bang."
- Chris,
a real chemist, on using Smart Tea instead of a paper lab book.

Making Tea

The Smart Tea project involves researchers from various fields within Chemistry and Computer Science. On the computer science team alone, we have researchers in semantic web information systems, grid computing, intelligent agents, web services, and human computer interaction.

In order for all of us to gain a better understanding of the chemistry lab experiences, and of the experimental design and execution process in particular, we made for a chemistry experiment. The experiment was led by team member Graham Smith, a chemist and computer scientist.



Background

When chemists those hypotheses for combining. For all its tech recorded using 200 years: a b. The flexibility: an experiment shelf. The book information at: for that matter completed: if t information is

Motivation

Part of the world wide [Semantic Grid](#) effort is to get the data crafted by individual scientists out of the lab and onto the Grid, where it can be accessed. The ancient concept of *paper* was of an invisible medium, all around us. In our concept of a lab author, the writer is the invisible medium holding information being generated within the lab. As chemists build up an experiment, they release the data to the lab author where it can be captured, stored and displayed in multiple contexts, from plain to publication.

We can think in terms of such an author now because of research developments like web services, intelligent agents and the semantic grid, the use effective information interaction design to support scientists both popular data into the author and grab it back as needed.

The Lab Author

With the evolution of the Semantic Grid and pervasive computing (information and computers everywhere), it is possible to change our thinking about information away from the lab book to the lab author.

The ancient concept of *paper* was of an invisible medium, all around us. In our concept of a lab author, the writer is the invisible medium holding information being generated within the lab. As chemists build up an experiment, they release the data to the lab author where it can be captured, stored and displayed in multiple contexts, from plain to publication.

We can think in terms of such an author now because of research developments like web services, intelligent agents and the semantic grid, the use effective information interaction design to support scientists both popular data into the author and grab it back as needed.

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"

[Trouble is...](#)

icists
gs for

Institute,

ic:
pages,

nd
pn) of this document.

or smouch)

Quinion for the explanation of smouch)

Semantic Chemistry II PNNL

20/07/2012

COSHH

Leverage off things we already have to do – "We have a cunning plan"

COSHH ASSESSMENT FORM			
SUBSTANCE NAME		PHYSICAL FORM	QUANTITY
Water		liquid	1000ml
Dextrose		Solid	<20g
Caffeine		Solid (brown)	<1g
Milk		liquid	<100ml
NATURE OF PROCESS		NATURE OF HAZARD	
liquid emulsion of caffeine, followed by combination with dextrose to produce a sweet drink		No specific hazardous substances? No # 20, why not use it?	
CONTROL MEASURES REQUIRED (Local exhaust, ventilation, personal protection, etc.)		No specific measure required	

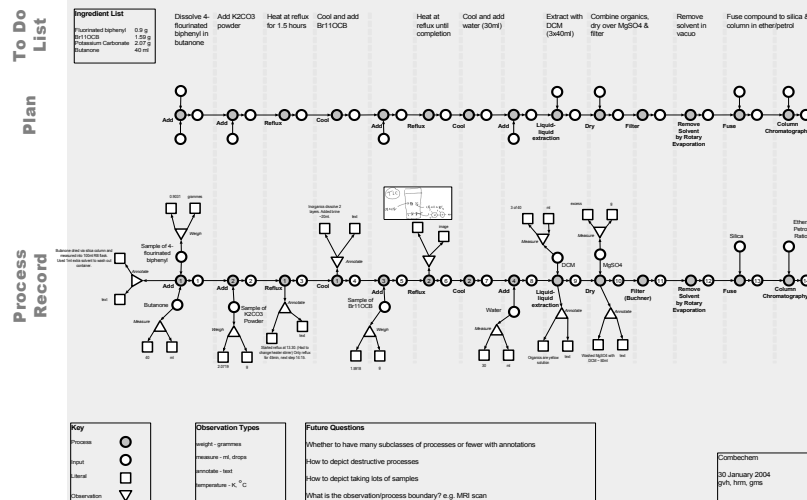
The fully semantic ELN - everything is linked!
Processes, materials and data

20/07/2012

Semantic Chemistry II PNNL



PLAN is a key ingredient to efficient and safe working



20/07/2012

Semantic Chemistry II PNNL

ELN In Application

Andrew Bailey
ajb302@soton.ac.uk

20/07/2012

Semantic Chemistry II PNNL

The Two Interfaces

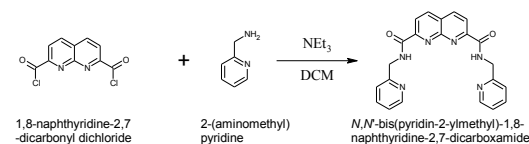
A Worked Example

Planning and Review

20/07/2012

Implementation

Semantic Chemistry II PNNL



Acid Chloride + Amine → Amide

20/07/2012

Semantic Chemistry II PNNL

The Planning Process

Materials

20/07/2012

Semantic Chemistry II PNNL

20/07/2012

Semantic Chemistry II PNNL

Procedure

N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarboxamide

ap0512555 (In Progress)

A Preparation of N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarboxamide

Materials

50.0 ml Dichloromethane
1.31 ml Triethylamine
1.1 g 1,8-Naphthyridine-2,7-dicarbonyl dichloride
0.97 ml 2-(aminomethyl)pyridine

Add material

Safety

1,8-Naphthyridine-2,7-dicarbonyl dichloride
R 40 Limited evidence of a carcinogenic effect. COSHH form checked

2-(aminomethyl)pyridine
Harmful in contact with skin and if swallowed. Causes burns. Density = 1.0489g/mL (2.2 eqv = 1.025g = 0.977 mL)

Dichloromethane
R 40 Limited evidence of a carcinogenic effect. COSHH form checked

Triethylamine
R 11 Highly flammable R 20/21/22 Harmful by inhalation, in contact with skin and if swallowed. R 35 Causes severe burns. (0.73 g/mL, 101.2 g/mol)

Procedure

1. The 1,8-Naphthyridine-2,7-dicarbonyl dichloride weighed out and placed in a round bottom flask

2. To this still dried Dichloromethane was added and the flask placed above a magnetic stirrer plate.

3. 2-(aminomethyl)pyridine is added dropwise via a needle and syringe

4. Following this the triethylamine was added dropwise

5. The reaction was left to stir overnight and was monitored by TLC

6. Once the TLC showed the completion of the reaction it was poured into 50 mL of water

7. The Organic layer was retained and was washed with further water (2 x 50 mL)

8. The organic layer was then washed with 50 mL of brine and the organic was then reduced in vacuo

9. The solid residue was then recrystallised from a DCM/diethylether mixed solvent system

10. The product was characterised

11.

20/07/2012

Semantic Chemistry II PNNL

Into the Lab!

N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarbonyl dichloride

ap0512555 (In Progress)

A Preparation of N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarbonyl dichloride

Materials

1,8-Naphthyridine-2,7-dicarbonyl dichloride
2-(aminomethyl)pyridine
Dichloromethane
Triethylamine

Status

0 of 4 materials have been measured.
0 of 10 steps have been completed.

Measure

Selected Material - 1,8-Naphthyridine-2,7-dicarbonyl dichloride

Atomic Weight
255.1

COSHH Information
Not Known, Treat as toxic

Amount
Required
1.1 g
Used
1.1483 g

Record Amount

20/07/2012

Semantic Chemistry II PNNL

Into the Lab!

N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarbonyl dichloride

ap0512555 (In Progress)

A Preparation of N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarbonyl dichloride

Materials

50.0 ml Dichloromethane (50.0 ml used)
1.31 ml Triethylamine (1.3 ml used)
1.1 g 1,8-Naphthyridine-2,7-dicarbonyl dichloride (1.1483 g used)
0.97 ml 2-(aminomethyl)pyridine (1.0 ml used)

Add material

Safety

1,8-Naphthyridine-2,7-dicarbonyl dichloride
R 40 Limited evidence of a carcinogenic effect. COSHH form checked

2-(aminomethyl)pyridine
Harmful in contact with skin and if swallowed. Causes burns. Density = 1.0489g/mL (2.2 eqv = 1.025g = 0.977 mL)

Triethylamine
R 11 Highly flammable R 20/21/22 Harmful by inhalation, in contact with skin and if swallowed. R 35 Causes severe burns. (0.73 g/mL, 101.2 g/mol)

Observe

Procedure - Step 7 of 10

Instructions

The Organic layer was retained and was washed with further water (2 x 50 mL)

Observations/Notes

This drew a little more colour off the organic layer and left it slightly cloudy and yellow

Draw **Write**

Next step >>

20/07/2012

Semantic Chemistry II PNNL

N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarbonyl dichloride

ap0512555 (In Progress)

A Preparation of N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarbonyl dichloride

Materials (4 of 4 measured)

50.0 ml Dichloromethane (50.0 ml used)
1.31 ml Triethylamine (1.3 ml used)
1.1 g 1,8-Naphthyridine-2,7-dicarbonyl dichloride (1.1483 g used)
0.97 ml 2-(aminomethyl)pyridine (1.0 ml used)

Add material

Safety

1,8-Naphthyridine-2,7-dicarbonyl dichloride
R 40 Limited evidence of a carcinogenic effect. COSHH form checked

2-(aminomethyl)pyridine
Harmful in contact with skin and if swallowed. Causes burns. Density = 1.0489g/mL (2.2 eqv = 1.025g = 0.977 mL)

Triethylamine
R 11 Highly flammable R 20/21/22 Harmful by inhalation, in contact with skin and if swallowed. R 35 Causes severe burns. (0.73 g/mL, 101.2 g/mol)

Procedure (9 of 10 steps complete)

1. The 1,8-Naphthyridine-2,7-dicarbonyl dichloride weighed out and placed in a round bottom flask

2. To this still dried Dichloromethane was added and the flask placed above a magnetic stirrer plate.

3. 2-(aminomethyl)pyridine is added dropwise via a needle and syringe

4. Following this the triethylamine was added dropwise

5. The reaction was left to stir overnight and was monitored by TLC

6. Once the TLC showed the completion of the reaction it was poured into 50 mL of water

7. The Organic layer was retained and was washed with further water (2 x 50 mL)

8. The organic layer was then washed with 50 mL of brine and the organic was then reduced in vacuo

9. The solid residue was then recrystallised from a DCM/diethylether mixed solvent system

10. The product was characterised

11.

20/07/2012

Semantic Chemistry II PNNL

Observations

Step 1

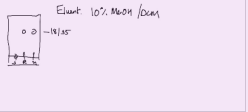
Step 2
gave a murky brown solution

Step 3
A white precipitate was formed as the amine was added to the reaction mixture

Step 4
As the triethylamine was added the white precipitate dissolved.

Step 5

Eluent: 10% MeOH / DCM
0.0 - 14/15



Overnight the reaction went purple with a gummy pot. By TLC reaction appears to have produced some product although it was impossible to confirm if the reaction has gone to completion, as the starting material(s) are too polar to elute. However the workup was continued as planned.

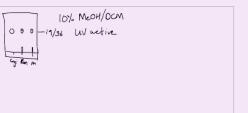
Step 6
This gave two layered separation, when shaken the aq layer (top) became red and the bottom layer was an off yellow

Step 7
This drew a little more colour off the organic layer and left it slightly cloudy and yellow

Step 8
This removed the cloudiness from the organic layer, and then it yielded a yellow solid. 1.283g

Step 9

10% MeOH / DCM
0.0 - 14/15 W. active



This was carried out as planned and yielded a yellow crystalline solid, 0.836g. Which appeared clean by TLC.

Step 10

56

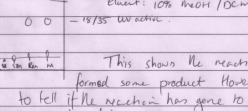
Actual mass of 1,8-naphthoquinone used: 1.843g

- Dissolution of the solid in DCM gave a murky brown solution.

- On addition of the amine, a white precipitate formed which dissolved again on addition of triethylamine.

After stirring overnight the reaction was TLC'd.

Eluent: 10% MeOH / DCM
0.0 - 14/15 W. active



This shows the reaction to have formed some product. However it is hard to tell if the reaction has gone to completion due to polarity of the SM.

The workup proceeded as followed:
Reaction poured into water (50ml) and separated.
The organic was washed with a further (2x50ml) this separated red from the organic and leave a cloudy yellowish solid.
This organic was then washed with 50ml of water.
This removed the cloudiness and left a yellow solid.
Vacuum dried (1.283g)
Recrystallized from DCM by other means to yield 0.836g of yellow solid.
Clean by NMR (H¹) and X-ray crystallography.

(C) University of Southampton IT Innovation Centre, 2009
 Copyright in this library belongs to the University of Southampton
 University Road, Highfield, Southampton, UK, SO17 1BJ
 This software may not be used, sold, licensed, transferred, copied
 or reproduced in whole or in part in any manner or form or in or
 on any media by any person other than in accordance with the terms
 of the Licence Agreement supplied with the software, or otherwise
 without the prior written consent of the copyright owners.
 This software is distributed WITHOUT ANY WARRANTY, without even the
 implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR
 PURPOSE, except where stated in the Licence Agreement supplied with
 the software.
 Created By : Ken Meacham
 Created Date : 2009/07/20
 Created for Project : moreTea
 Dependencies : none
 <!DOCTYPE rdf:RDF [
 <ENTITY rdf 'http://www.w3.org/1999/02/22-rdf-syntax-ns#>
 <ENTITY rdfs 'http://www.w3.org/2000/01/rdf-schema#>
 <ENTITY xsd 'http://www.w3.org/2001/XMLSchema#>
 <ENTITY base 'http://schemas.it-innovation.soton.ac.uk/moretea/experiment/0.2/rdf-
 schema#>
 <ENTITY experiment '&base;#>
]>

P&E

Peony



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

“The oreChem Project

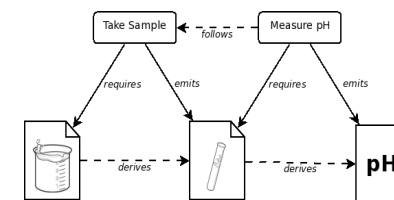
“An ontology for Planning and Enactment”

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

Unknown (possibly Yogi Berra)

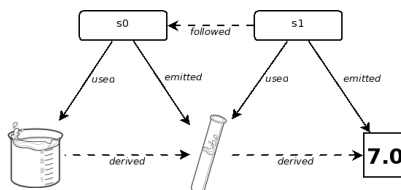
P&E Ontology: Planning

- 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

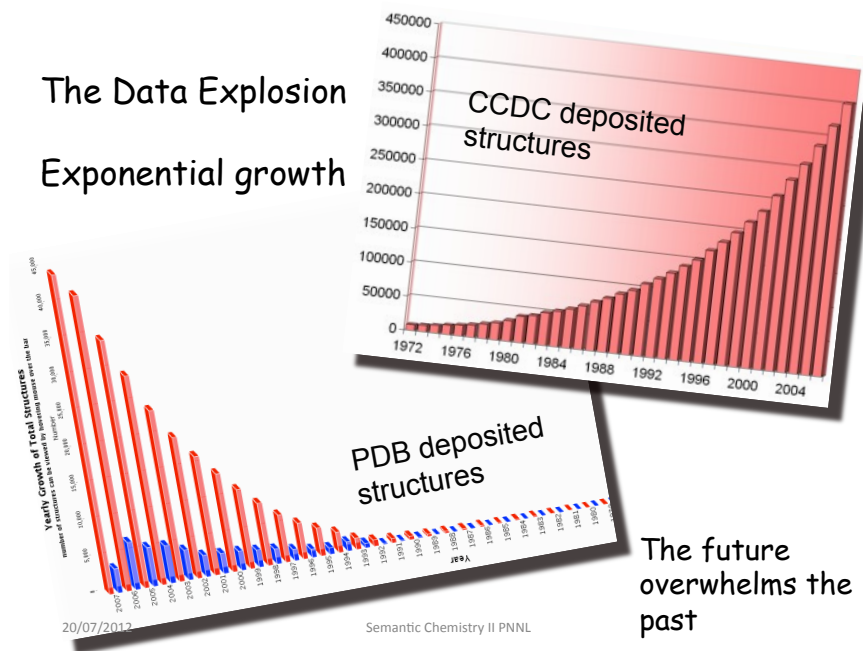


20/07/2012

Semantic Chemistry II PNNL

The Data Explosion

Exponential growth



20/07/2012

Semantic Chemistry II PNNL

Unavailable Information

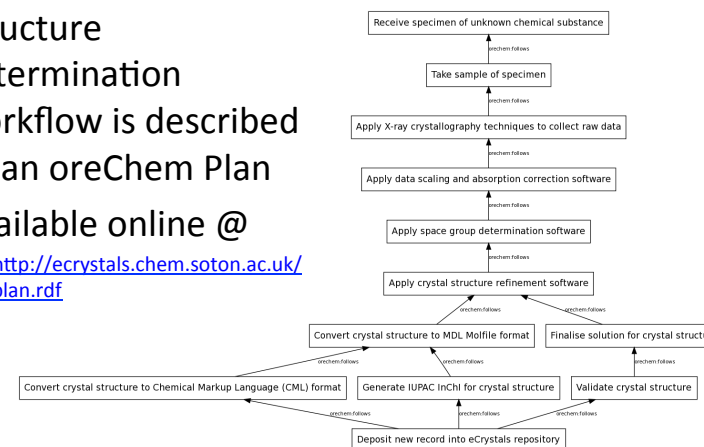
- Not just lots of data but why are many of the structures unpublished so certainly unavailable?
- The E-Crystals and E-Bank Project looked at how to address this issue
- Is making data available the same as depositing a copy with someone else?

20/07/2012

Semantic Chemistry II PNNL

oreChem Plan for eCrystals

- Structure determination workflow is described by an oreChem Plan
- Available online @
 - <http://ecrystals.chem.soton.ac.uk/plan.rdf>



20/07/2012

Semantic Chemistry II PNNL

Human AND Computer Readable

Southampton University

eCrystals

Home | About | Browse by Year | Browse by People

Login | Create Account

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

Chemical Formula: $C_{14}H_{20}O_5$

Identifiers: $14H-14H-5$

Identifiers: $14H-14H-5$

Control Number: $14H-14H-5$

Deposit: $14H-14H-5$

Depositor: $14H-14H-5$

Structure: $14H-14H-5$

Data collection: $14H-14H-5$

Chemical structure: $14H-14H-5$

Stages (10)

Stage: 1 plan.rdf

Stage: 2 plan.rdf

Semantic Chemistry

20/07/2012

XHTML

Mark's Blog

Southampton University

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

Chemical Formula: $C_{14}H_{20}O_5$

Identifiers: $14H-14H-5$

Identifiers: $14H-14H-5$

Control Number: $14H-14H-5$

Deposit: $14H-14H-5$

Depositor: $14H-14H-5$

Structure: $14H-14H-5$

Data collection: $14H-14H-5$

Chemical structure: $14H-14H-5$

Stages (10)

Stage: 1 plan.rdf

Stage: 2 plan.rdf

Semantic Chemistry

20/07/2012

XHTML with RDFa

Mark's Blog

Southampton University

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

Chemical Formula: $C_{14}H_{20}O_5$

Identifiers: $14H-14H-5$

Identifiers: $14H-14H-5$

Control Number: $14H-14H-5$

Deposit: $14H-14H-5$

Depositor: $14H-14H-5$

Structure: $14H-14H-5$

Data collection: $14H-14H-5$

Chemical structure: $14H-14H-5$

Stages (10)

Stage: 1 plan.rdf

Stage: 2 plan.rdf

Semantic Chemistry

20/07/2012

20/07/2012

Semantic Chemistry II PNNL

RSC Publishing Blogs Home

Sample Originator: Michael B. Hursthouse, Simon J. Coles, G. McKimming and Mark E. Light

Chemical Formula: $C_{22}H_{25}N_3O_3$

Identifiers: $14H-14H-5$

Identifiers: $14H-14H-5$

Control Number: $14H-14H-5$

Deposit: $14H-14H-5$

Depositor: $14H-14H-5$

Structure: $14H-14H-5$

Data collection: $14H-14H-5$

Chemical structure: $14H-14H-5$

Stages (10)

Stage: 1 plan.rdf

Stage: 2 plan.rdf

Semantic Chemistry

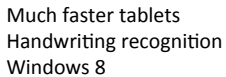
20/07/2012

Making use of publicly available Chemistry Services

BRINGING THE PARTS TOGETHER

20/07/2012

Semantic Chemistry II PNNL



Semantic Chemistry II PNNL



Semantic Chemistry II PNNL

Semantic Chemistry II PNNL

Grid-based dynamic electronic publication: a case study using combined experiment and simulation studies of crown ethers at the air/water interface

Esther R Rousay, Hongchen Fu, Jamie M Robinson, Jonathan W Essex and Jeremy G Frey

Phil. Trans. R. Soc. A 2005 **363**, 2075-2095
doi: 10.1098/rsta.2005.1630

20/07/2012

Semantic Chemistry II PNNL

R/LISP Papers

P <- read("http://eprints.soton.ac.uk/frey/reproducible.computable.paper")

Summary(p)

Abstract(p) vs p\$Abstract {First abstracts the paper, second gives the papers' abstract}

p\$Title

Print(p\$Text); variables <- p\$Quantities

Graph <- p\$Graphs or to access the data in the graph p\$Graphs\$Table\$Quantities

Context(P)

Context(P) <- New.Context(new_thermodynamic_data)

p1 <- Run(p) ; run with new context : value of $\Delta_r H(\text{OH})$

Diff <- p - p1 ; what conclusions change

Quantity	Names
	Symbol
	Value
	Units
	Prov

UNIVERSITY OF HAMPTON

This Post

Permalink

URI

Label

Revisions

Export:

XML (With Files)

PNG image

This Blog

New Post

Blog Settings

Timeline View

Export Blog

Archives

November 2011 (18)

Frey & DeRoure

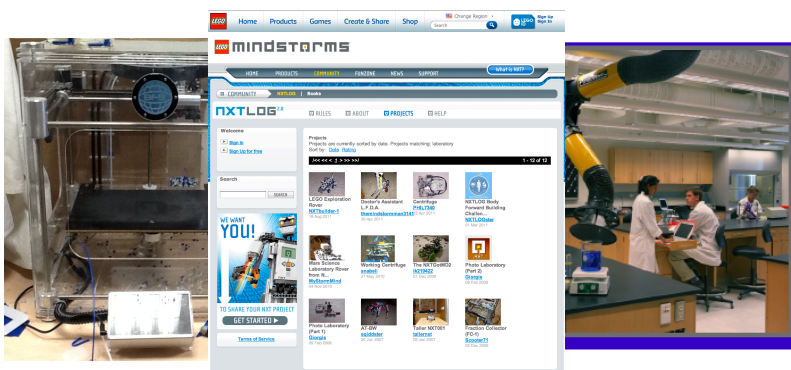
Stockholm

4t Paradigm Next Step

meeting

4 Dec 2011

Change in the whole way we design and build



3D Printers

Shared Space?

20/07/2012

Semantic Chemistry II PNNL

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

20/07/2012

Semantic Chemistry II PNNL

Thanks

- UK e-Science Programme
- RCUK, EPSRC, JISC, BBSRC, HEFCE, Microsoft & IBM, for funding
- Southampton Colleagues and Students from Chemistry, Electronics & Computer Science, Engineering, Mathematics, iSolutions and the Library
- Colleagues at UKOLN, STFC, University of Reading
- Colleagues from Penn State, Cornell, PNNL, UNSW, USyd



20/07/2012

Semantic Chemistry II PNNL

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

re collection. All rights reserved.
re the Bank of Technology Caricatures.