

New Web-based Approaches to Communicating and Teaching in Chemistry & Crystallography

Simon Coles

EPSRC National Crystallography Service

School of Chemistry

University of Southampton



@malaria

blogs@ChemTools
The thoughts of Chemists

my experiment^{beta}

“The internet wasn't created for mockery! It was created so scientists from different universities could share datasets...”

Simpson, H. *The Simpsons* (2005), Eds. Groening, M., Brooks, J.L. & Simon, S., Series 16, Episode 8, Original air date (US) 06-Feb-2005.

<http://www.tvtome.com/tvtome/servlet/GuidePageServlet/showid-146/epid-346864/>

Social Networks for Chemists



The screenshot shows the nanoHUB website, a platform for nanoscience and technology. The header features the nanoHUB logo and a search bar. The main content area displays a series of lectures titled 'Nanotechnology 101' and 'Nanotechnology 501'. Below these, sections for 'Simulate', 'Research', 'Teach & Learn', and 'Contribute' are visible, each with sub-options and icons. A sidebar on the left lists tools for Nanoelectronics, NEMS/Nanofluidics, and Nano-Bio Devices. The footer includes a 'Help' link and the NCN logo.

nanohUB
online simulation and more

Home My nanoHUB Resources Contributors Events About Support

Search

Help

Nanotechnology 101
Introduction to nanotechnology

Nanotechnology 101 is a series of lectures designed to provide an undergraduate level introduction to nanotechnology. Our Nanotechnology 501 series offers lectures directed at the graduate student/ professional level.

Learn more

A resource for nanoscience and technology, the nanoHUB was created by the NSF-funded NCN and its development is driven by research themes in:

Nanoelectronics **new**
NEMS/Nanofluidics
Nano-Bio Devices

NCN

Simulate

- Nanoelectronics Tools for nanoelectronics
- NEMS/Nanofluidics Tools for NEMS and Nanofluidics
- Nano-Bio Devices Tools for nano-bio devices
- More > Browse all available tools

Research

- Seminars Browse research seminars
- Collaborate Work with your colleagues
- Web Meetings Right in your browser
- User Groups Share with your colleagues

Teach & Learn

- Nano 101 / Nano 501 Introductory tutorials
- Nanocurriculum Curriculum on Nanoelectronics
- Learning Modules Self-paced web instruction
- Teaching Materials Graduate, Undergrad, K-12

Contribute

- Contribute Content Upload your own materials
- Give us Feedback Success story? Suggestions?
- Take a Poll What aggregator do you use for RSS feeds?
- Donations Contribute your financial support

Google generation: new behaviour and approach

Sharing Rich Media

The image shows a 3D rendering of a tablet displaying a hybrid video and paper publication on the SciVEE platform. The screen shows a video of a lab experiment and a linked paper abstract.

SciVEE beta

browse **upload** **community**

Take a Tour **Tutorials** **Help**

pubcasts **videos** **channels** **tags**

UCSD Organic Lab: Recrystallization

Submitted by: joshuakrohn

Description: For further details about UCSD Professor Haim Weizman's organic lab and classes please visit: http://chem-courses.ucsd.edu/CoursePages/Uglabs/143A_Weizman/

Rating: ★★★★★

JOVE JOURNAL OF VISUALIZED EXPERIMENTS

Welcome **Browse** **Submit**

Click Here to Search

Email/Alias **I am new...** **Password** **I forgot...** **Sign In**

Encountered a problem? Please let us know.

ISSN 1940-087X

Publish With Us!
We are accepting submissions.

If I Can't Make Videos...
It's ok: JOVE can send a professional videographer to film your experiment.

Does it Take a Long Time?
Not at all. On average, filming takes 3 to 4 hours.

How do I start?
[Click here](#) to begin your submission or [send us an email](#).

Resource Videos

Editor's Picks

06/27/2008 **Isolation of Early Hematopoietic Stem Cells from Murine Yolk Sac and AGM**

07/02/2008 **Whole-cell Recordings of Light Evoked Excitatory Synaptic Currents in the Retinal Slice**

04/09/2008 **Resource Article: The RosetteSep® Kit from STEMCELL Technologies**

08/15/2008 **Generation of Stable Transgenic *C. elegans* Using Microinjection**
Laura A. Berkowitz, Adam L. Knight, Guy A. Caldwell, Kim A. Caldwell
Department of Biological Sciences, University of Alabama

This video demonstrates the technique of microinjection into the gonad of *C. elegans* to create transgenic animals.

08/14/2008 **Imaging Effector Memory T cells in the Ear After Induction of Adoptive DTH**
Melanie P. Matheu¹, Christine Beeton¹, Ian Parker², K. George Chandy¹, Michael D. Cahalan¹
¹Department of Physiology and Biophysics, University of California, Irvine, ²Department of Neurobiology and Behavior, University of California, Irvine

Here we demonstrate a method for inducing and recording the progress of a delayed type-hypersensitivity (DTH) reaction in the rat ear. This is followed by a demonstration of the preparation of rat ear tissue for two-photon imaging of the effector / memory T cell response.

View Protocol >>

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View Protocol >>

• Video + Paper = Pubcast

New Approaches to ‘Sharing Experiments’



- Specialised domain-oriented innovations

Formation of Open Communities

The screenshot shows a list of member laboratories on the OpenWetWare website. The laboratories are categorized by continent:

- Europe**
 - [Universiti Teknologi Malaysia \[show\]](#)
 - [Bristol University \[show\]](#)
 - [CeMM \(Vienna\) \[show\]](#)
 - [CNRS \[show\]](#)
 - [Cambridge Research Institute \[show\]](#)
 - [ETH Zurich, Switzerland \[show\]](#)
 - [FH Campus Wien \[show\]](#)
 - [Imperial College \[show\]](#)
 - [King's College London \[show\]](#)
 - [Norwich Research Park, UK \[show\]](#)
 - [PRBB \[show\]](#)
 - [Technische Universiteit Delft \[show\]](#)
 - [Univ of Cambridge \[show\]](#)
 - [Univ of Edinburgh \[show\]](#)
 - [Univ of Ljubljana \[show\]](#)
 - [Univ of Manchester, UK \[show\]](#)
 - [MH Hannover, Germany \[show\]](#)
 - [Univ Paris 5-INserm \[show\]](#)
- Oceania**
 - [CAMBIA \[show\]](#)
 - [Univ of Otago \[show\]](#)
- Labs in development**
 - [Labs in development \[show\]](#)

Each entry includes a link to edit the page. To the right, a call-to-action box encourages users to add their lab to the community:

Add your lab to OWW [edit]

Interested in starting a lab wiki on OpenWetWare? See the [starting a lab wiki tutorial](#)

- New approaches surfacing and growing FAST

Open Notebook Science

Useful Chemistry

Google Custom Search

Search

This is an open source science project in chemistry. Post specific problems in chemistry that Post specific partial solutions to these problems. Or execute a suggested step. NOTE: ANYTHING SUBJECT TO A SHARE-ALIKE WITH ATTRIBUTION CREATIVE COMMONS LICENSE (see bottom of page).

UsefulChem

Exp025 Protected page discussion history notify

Oc1ccc(OCCNCC)cc1 $\xrightarrow[\text{116-118 } \text{C}_1 \text{ 1h}]{\text{H}_3\text{PO}_4}$ Oc1ccc(O)cc1

Objective
To convert [adrenaline](#) to [DOPAL](#) by acid catalysis

Procedure
A solution of [adrenaline](#) (1.0g 5.5mmoles) in 85% phosphoric acid was heated (116-118°C for 1h) in a heating mantle then removed from heat and allowed to cool. The solution was stirred for 1h, then saturated with NaCl. It was taken up in ethyl ether, and dried over anhydrous MgSO₄. The ether was then removed to obtain DOPAL (80 mg 0.53mmol, 9.5% yield)

Characterization:

Results

1. [TLC of 25A in 3:1 MeCl₂/MeOH](#) and in [5:1 MeCl₂/MeOH](#), and [stained with CAM](#)
2. [HNMR of 25A](#) in acetone-d₆, and the expansions of the prominent peak regions ([one](#) Varian inova). The integration is good enough to not require further purification.

Discussion
This is the first time that DOPAL was obtained pure (by NMR integration) immediately after heating. There are several factors that may have contributed to this: preheating the phosphoric acid then adding the reaction under nitrogen and a careful temperature control. It is likely that the main impurity in previous attempts (Exp016, Exp023) is the carboxylic acid ([Exp016HNMR](#), [Exp023HNMR](#)).

Conclusion
DOPAL can be obtained pure in 9.5% yield by heating adrenaline in 85% phosphoric acid, hydrolysis and extraction into ether.

s Page

Home Research CV Publications My Life Contact

I've decided to give Open Notebook Science a try. My lab notebook is pretty large (30MB, 350+ pages), so it may take a while to download.

[download my lab notebook](#)

Other Open Science Notebooks
Jean-Claude Bradley maintains a list of [Open Science Notebooks](#). If you decide to make your lab notebook open, send him an email to be put on the list so others can find your work more easily.

Help me improve my notebook
I'm also trying to come up with some [Open Notebook Science requirements and suggestions](#) to help move towards an open notebook that is intelligible to people besides myself. I'd be interested for your comments/suggestions on what else should be included.

How I construct my notebook
A few people have written asking how I make the document itself. The document is made in latex (specifically pdflatex). I've posted a simple [example electronic lab notebook in latex](#) with the commands and functions that I use. sample.tex is the compiled document. If you don't have latex installed, you can use [pdflatex](#) to convert the sample.tex file into a pdf. I've also posted an [Introduction to Latex](#).

RR RESEARCH
THINKING ABOUT OUR RESEARCH INTO THE MECHANISM, FUNCTION AND EVOLUTION OF DNA UPTAKE BY HAEMOPHILUS INFLUENZAE AND OTHER BACTERIA.

SATURDAY, JANUARY 19, 2008

ABOUT ME

ROSIE REDFIELD
CANADA
I run a microbiology research lab in the Life Sciences Centre at the University of British Columbia.

VIEW MY COMPLETE PROFILE

PREVIOUS POSTS

- Thermodynamics of home heating
- Gene transfer agent
- Sorry, wrong link
- Sorry for the paucity of posts
- Genespring progress and problems
- Data on *E. coli* protein

POSTED BY ROSIE REDFIELD AT 6:25 PM

2 COMMENTS:

iayork said...

Remember what you've said about sxy in the past. Can you make a null version of

- Immediate sharing of experimental information & data

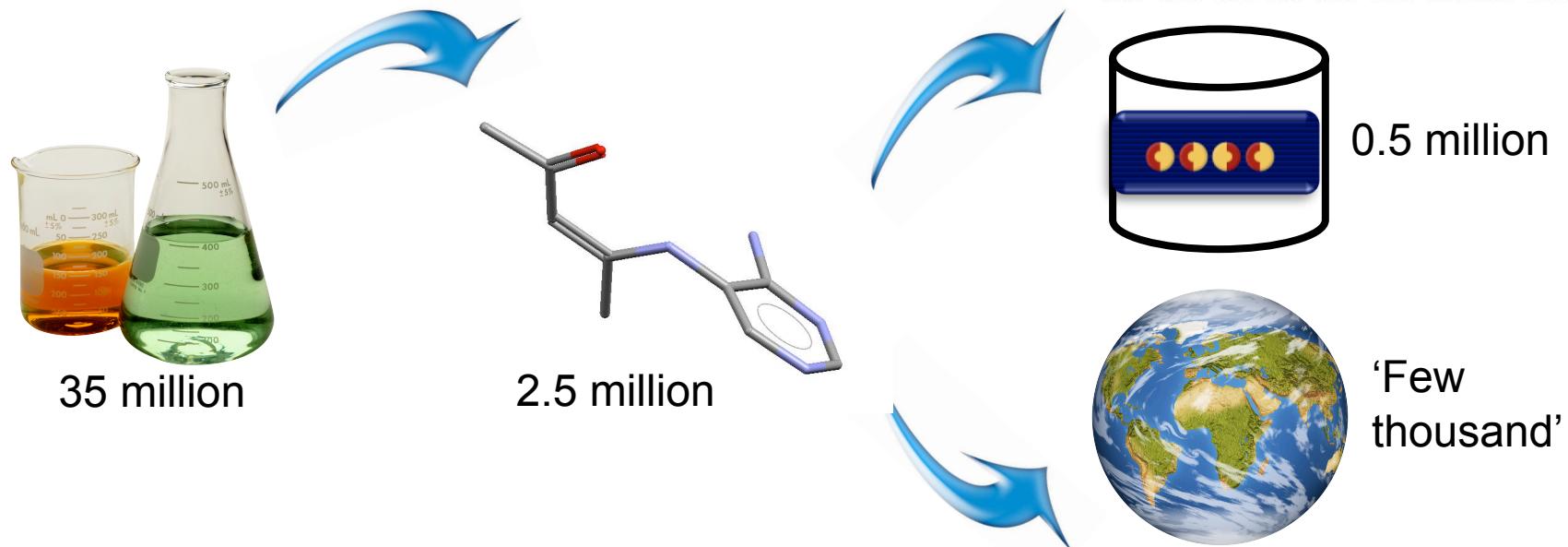
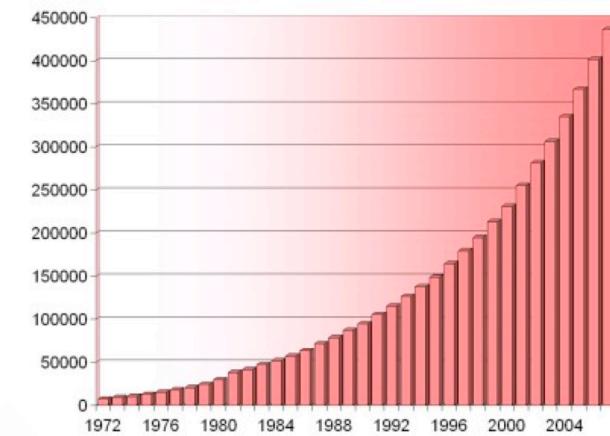
New Information Exchange Environments



- Immersive alternative to conventional browsing & interaction

Data Deluge

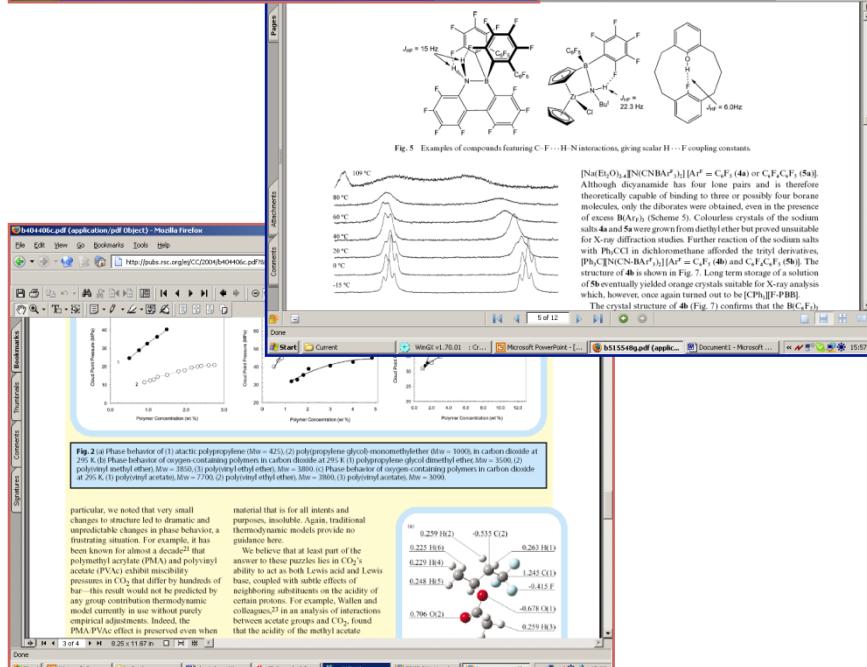
- 40 years ago a PhD student would determine about 3 crystal structures for their thesis – this can now be easily achieved in a day



The primary cause is the current data publication process, which is tied to journal articles and peer review

The Solution

Intellect & Interpretation (Journal article, report, etc)

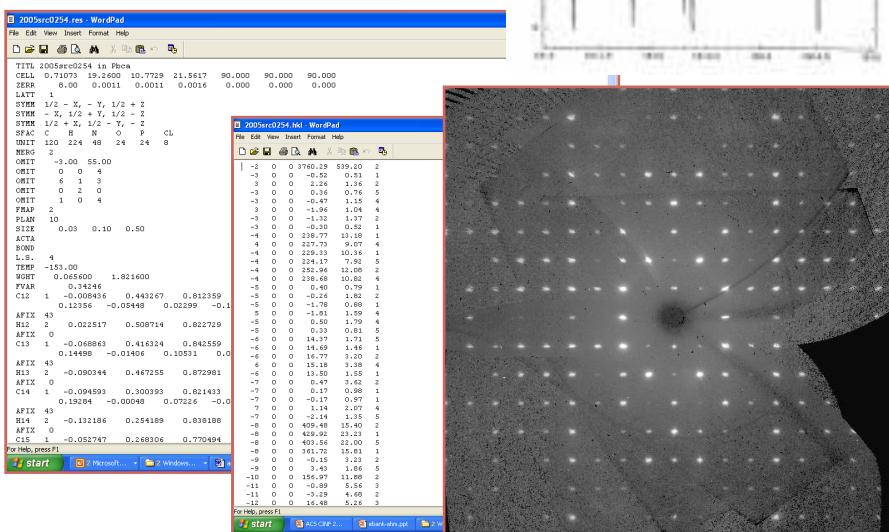
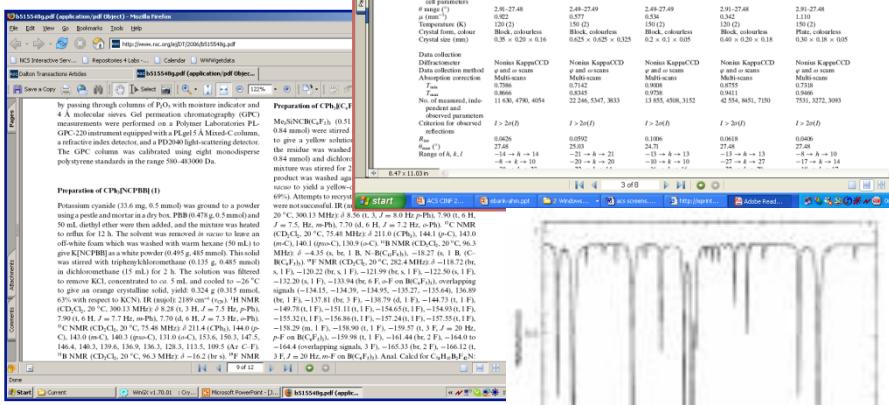


particular, we noted that very small changes to structure led to dramatic and unpredictable changes in phase behavior, a frustrating situation. For example, it has been known for almost 20 years that poly(methyl acrylate) (PMA) and polyvinyl acetate (PVA) exhibit miscibility in CO_2 , that is, they can be miscible by any group contribution thermodynamic approach.²³ However, when PMA/PVA blend is preserved even when

material that is for all intents and purposes, insoluble. Again, traditional thermodynamic models provide no guidance here.

We note that at least part of the answer to these puzzles lies in Lewis' ability to act as both Lewis acid and Lewis base, coupled with subtle effects of high-temperature phase behavior of certain proton. For example, Wallen and colleagues²³ in a analysis of interactions between acetate groups and CO_2 found the acidity of the methyl acetate

Underlying data (Institutional data repository)



The eCrystals Data Repository

 **eCrystals** UNIVERSITY OF Southampton

Home | About | Browse by Year | Browse by People | [Manage deposits](#) | [Profile](#) | [Saved searches](#) | [Review](#) | [Admin](#) | [Logout](#) | | [Search](#)

Logged in as Dr Richard A Stephenson | [Manage deposits](#) | [Profile](#) | [Saved searches](#) | [Review](#) | [Admin](#) | [Logout](#)

2,2-trimethylenedioxy-4,4,6,6-tetrachlorocyclotriphosphazene

Sample Originator: A. Kilic^a, M. Odlyha^b, A. Uslu^a, David B. Davies^b and R.A. Shaw^b.

Data Collection: Mark E. Light^a, Simon J. Coles^a and Susanne. L. Huth^a

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

Gebze Institute of Technology^a
Birkbeck College^b
University of Southampton^a

C3H6Cl4N3O2P3
InChI=1/C3H12Cl4N3O2P3/c4-13(5)8-14(6,7)10-15(9-13)11-2-1-3-12-15/h8-10,13-15H,1-3H2

Identification Number: 10.3737/ecrystals.chem.soton.ac.uk/300

Controlled keywords: cyclophosphazene, phase transition, variable temperature

Date: 28 March 2007
Created:
Deposited On: 21 Apr 2008 15:56
Deposited By: Dr Simon J Coles

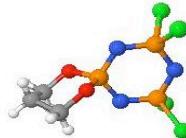
Data collection parameters

Chemical formula	C3 H6 Cl4 N3 O2 P3
Crystallisation Solvent	
Crystal morphology	Rod
Crystal system	Orthorhombic
Space group symbol	Pna2(1)
Cell length a	13.4804(14)
Cell length b	10.6442(9)
Cell length c	8.8479(7)
Cell angle alpha	90.00
Cell angle beta	90.00
Cell angle gamma	90.00
Data collection temperature	274(2)

Refinement results

Solution figure of merit	0.0569
R Factor (Obs)	0.0334
R Factor (All)	0.0380
Weighted R Factor (Obs)	0.0871
Weighted R Factor (All)	0.0905

Citation: Kilic, A. and Odlyha, M. and Uslu, A. and Davies, David B. and Shaw, R.A. and Light, Mark E. and Coles, Simon J. and Huth, Susanne. L. and Hursthouse, Michael B. and Rutherford, J.S. (2007) University of Southampton, Crystal Structure Report Archive. ([doi:10.3737/ecrystals.chem.soton.ac.uk/300](http://10.3737/ecrystals.chem.soton.ac.uk/300)) Export as: [EndNote](#) [BibTeX](#) [ASCII Citation](#)



Available Files

Final Result	
2005sjc0007.cif	11k
2005sjc0007.cml	4k
2005sjc0007.fcf	138k
Validation	
2005sjc0007_checkcif.htm	9k
Refinement	
2005sjc0007.res	5k
2005sjc0007_xl.lst	29k
Solution	
2005sjc0007.ppr	5k
2005sjc0007_xs.lst	44k
Processing	
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2005sjc0007.htm	11k
2005sjc0007_0kl.jpg	91k
2005sjc0007_h01.jpg	87k
2005sjc0007_hk0.jpg	79k
Data Collection	
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Other Files	
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2005sjc0007.inchi	1k
2005sjc0007.ins	4k
2005sjc0007.mol	2k
2005sjc0007.p4p	1k
2005sjc0007_ellipsoid.gif	21k

- Quick & simple to deposit
- Software tools
- Laboratory archive
- Community involvement
- ‘Embargo’ facility
- Structured foundations
- Discoverable & harvestable



<http://ecrystals.chem.soton.ac.uk>

A Thorough Approach to Dissemination

- Using simple Dublin Core protocol (OAI-PMH)
 - Crystal structure
 - Title (Systematic IUPAC Name)
 - Authors
 - Affiliation
 - Creation Date
- Additional **chemical** information through Qualified Dublin Core
 - Empirical formula
 - International Chemical Identifier (InChI)
 - Compound Class & Keywords
- Specifies which 'datasets' are present in an entry
- Application Profile <http://www.ukoln.ac.uk/projects/ebank-uk/schemas/>
- DOI links <http://dx.doi.org/10.1594/ecrystals.chem.soton.ac.uk/145>
- Rights & Citation <http://ecrystals.chem.soton.ac.uk/rights.html>



eCrystals



Chem_XSeer



RSC



ChemistryCentral



Unilever Cambridge

Centre For Molecular Science Informatics



The University of Sydney

Reciprocal Net



UNIVERSITY OF
OXFORD

UNIVERSITY OF Southampton

eCrystals



Useful Chemistry



D|C|C



eBank UK

CrystalEye (beta)



Chemical Database Service

JISC

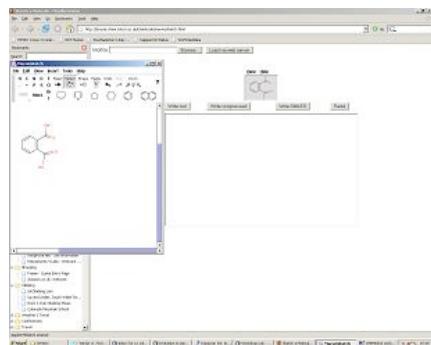


Engineering and Physical Sciences
Research Council

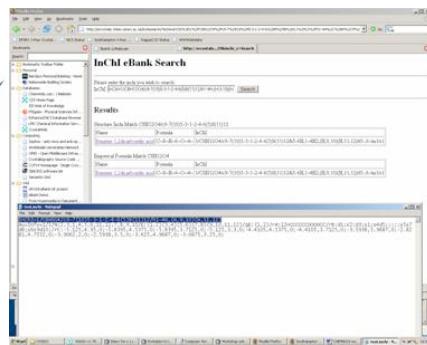
Poster (Thurs/Fri): P24.02.04 (C627)

Simple Integration into Teaching

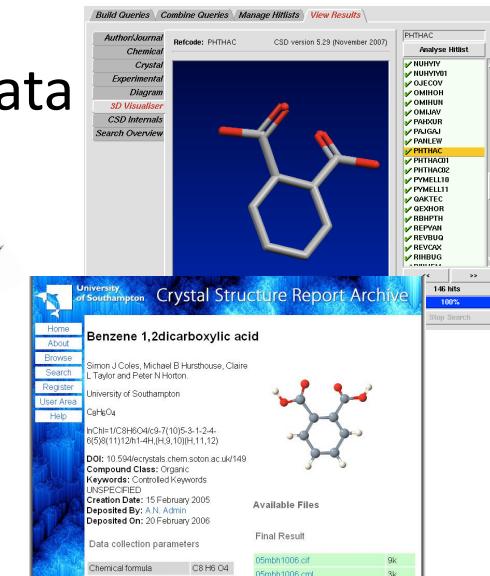
- Component of MChem course...using REAL data



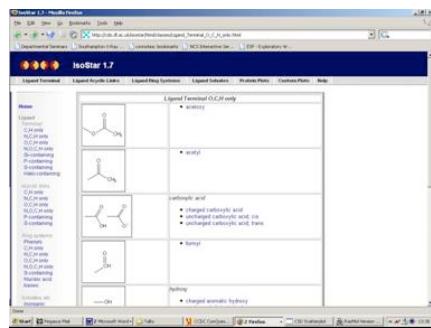
Devise



Search

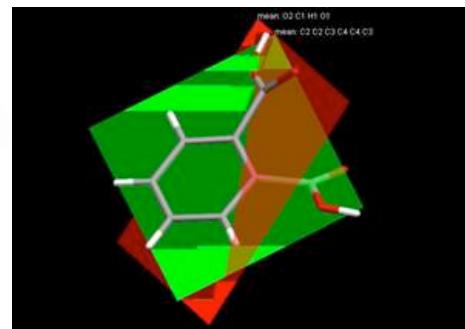


Discover

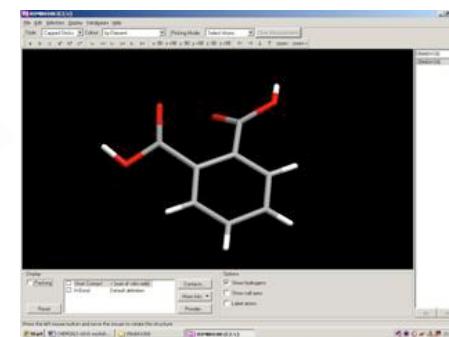
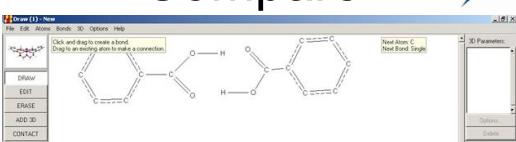


Compare

Analyse



Manipulate



Open Science Experiment

eCrystals UNIVERSITY OF Southampton

Home | About | Browse by Year | Browse by People | Login | Create Account | Search

N-(4-methylphenyl)acetamide

Sample Originator: Terry L. Threlfall^a.
Data Collection: Susanne L. Huth^a.
Structure Determination: Susanne L. Huth^a, Michael B. Hursthouse^a and Simon J. Coles^a.
University of Southampton^a
C9H11N
InChI=1/C9H11NO/c1-7-3-5-9(6-4-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)
Identification 10.3737/ecrystals.chem.soton.ac.uk/544
Number:
Controlled para-substituted acetanilide
Keywords:
Date 21 June 2008
Created:
Deposited 01 Aug 2008 17:29
On:
Deposited Ms L.S. Huth
By:
Data collection parameters
Chemical formula C9 H11 N O

Available Files

Final Result	2008ish008.cif	11k
	2008ish008.cml	3k
	2008ish008.fcf	89k

Validation
2008ish008_checkcif.htm 7k

eCrystals UNIVERSITY OF Southampton

Home | About | Browse by Year | Browse by People | Login | Create Account | Search

N-(4-methoxyphenyl)acetamide

Sample Originator: Terry L. Threlfall^a.
Data Collection: Susanne L. Huth^a.
Structure Determination: Susanne L. Huth^a, Michael B. Hursthouse^a and Simon J. Coles^a.
University of Southampton^a
C9H11NO2
InChI=1/C9H11NO2/c1-7(11)10-8-3-5-9(12-2)6-4-8/h3-6H,1-2H3,(H,10,11)
Identification 10.3737/ecrystals.chem.soton.ac.uk/543
Number:
Controlled para-substituted acetanilide
Keywords:
Date 21 June 2008
Created:
Deposited 01 Aug 2008 17:24
On:
Deposited Ms L.S. Huth
By:
Data collection parameters
Chemical formula C9 H11 N O 2

Available Files

Final Result	2008ish013.cif	11k
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	2008ish013.fcf	95k

Validation
2008ish013_checkcif.htm 7k

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Home | About | Browse by Year | Browse by People | Login | Create Account | Search

N-(4-ethoxyphenyl)acetamide

Sample Originator: Terry L. Threlfall^a.
Data Collection: Susanne L. Huth^a.
Structure Determination: Susanne L. Huth^a, Michael B. Hursthouse^a and Simon J. Coles^a.
University of Southampton^a
C10H13NO2
InChI=1/C10H13NO2/c1-3-13-10-6-4-9(5-7-10)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)
Identification 10.3737/ecrystals.chem.soton.ac.uk/547
Number:
Controlled para-substituted acetanilide
Keywords:
Date 07 July 2008
Created:
Deposited 01 Aug 2008 17:45
On:
Deposited Ms L.S. Huth
By:
Data collection parameters
Chemical formula C10 H13 N O 2

Available Files

Final Result	2008ish032.cif	11k
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	2008ish032.fcf	104k

Validation
2008ish032_checkcif.htm 7k

Refinement

eCrystals UNIVERSITY OF Southampton

Home | About | Browse by Year | Browse by People | Login | Create Account | Search

N-(4-methoxyphenyl)acetamide

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Structure Determination: Susanne L. Huth^a, Michael B. Hursthouse^a and Simon J. Coles^a.
University of Southampton^a
C9H11NO2
InChI=1/C9H11NO2/c1-7(11)10-8-3-5-9(12-2)6-4-8/h3-6H,1-2H3,(H,10,11)
Identification 10.3737/ecrystals.chem.soton.ac.uk/543
Number:
Controlled para-substituted acetanilide
Keywords:
Date 21 June 2008
Created:
Deposited 01 Aug 2008 17:24
On:
Deposited Ms L.S. Huth
By:
Data collection parameters
Chemical formula C9 H11 N O 2

Available Files

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Validation
2008ish013_checkcif.htm 7k

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University of Southampton^a
C10H13NO2
InChI=1/C10H13NO2/c1-3-13-10-6-4-9(5-7-10)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)
Identification 10.3737/ecrystals.chem.soton.ac.uk/547
Number:
Controlled para-substituted acetanilide
Keywords:
Date 07 July 2008
Created:
Deposited 01 Aug 2008 17:45
On:
Deposited Ms L.S. Huth
By:
Data collection parameters
Chemical formula C10 H13 N O 2

Available Files

Final Result	2008ish032.cif	11k
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	2008ish032.fcf	104k

Validation
2008ish032_checkcif.htm 7k

<http://ecrystals.chem.soton.ac.uk/544/>
<http://ecrystals.chem.soton.ac.uk/543/>
<http://ecrystals.chem.soton.ac.uk/547/>

Susanne Huth Talk (Sat):
MS.98.3 (C163)

eMalaria: Drug Discovery by School Children

Welcome to the e-malaria Project!

What's the problem?

Malaria kills over a million people a year, and it's spreading. The world needs new drugs to combat the disease. As resistance to existing drugs grows and global warming increases the range of the mosquito that need is increasing.

So what has this got to do with you?

Well we need you to design the drugs! This project asks you to design a small polypeptide, which we run a series of calculations on to determine its possible use as an anti-malarial drug. At this stage only four schools are signed up as pilot centres for the project. That means you are one of only about 100 people taking part in the project. You have a huge ability to effect the outcomes of the project at this stage.

What's in it for you?

Well we've provided some materials for you connected with the science involved in the project, which should help with revision. There are also opportunities for visits to Southampton and in school talks from project members. But the best thing by far is you could discover a brand new drug. The project has the ability to get promising compounds

The Drug Design Process

Step 1

Drug design is a long complicated process. It takes approximately 15 years to get a drug from concept to market, and it costs a staggering 350 million pounds. From somewhere in the region of 10,000 candidates only one drug will make it to the shops. So what happens that costs so much, and takes so long?

Step 2

The first thing is to determine the receptor pathway? Block hypothesis for treatment, how treatments are designed for cold and flu treatment, how to improve on existing treatments.

Step 3

The next question is how receptor pathway? Block hypothesis for treatment, how treatments are designed for cold and flu treatment, how to improve on existing treatments.

BBC Home

Last Updated: Wednesday, 22 June, 2005, 07:43 GMT 08:43 UK

[E-mail this to a friend](#) [Printable version](#)

Students to aid malaria research

School and college science students are being called on to help come up with a drug that could fight malaria.

The universities of Southampton and Reading have set up a website on the subject, primarily as a learning tool.

But their scientists say any A-level students that use the information to come up with a potential cure may have their drug compound tried out for real.

A spokesman for the scheme said: "This isn't just another teaching exercise this is a real life problem."

Students who register with The Schools Malaria Project website will be able to research the different ways of combating malaria.

We believe that there is a very real chance that some of the compounds that they come up with will be made

SEE ALSO:

- Fungus 'may help malaria fight'
- Malaria drug resistance warning
- Science shows how malaria 'hides'
- Global toll of malaria 'doubled'

RELATED BBC LINKS:

- Malaria - Global Menace

Bonding Dipoles

Dipoles are two equal and opposite partial charges on molecules. They arise from polar bonds. As opposite charges attract and like charges repel, dipoles can attract or repel each other depending on the types of dipole involved, and the way they are arranged. The following interactions are possible:

- Permanent dipole - permanent dipole
- Permanent dipole - induced dipole
- Temporary dipole - induced dipole

These are only a few of the possible interactions between a drug molecule and its target. Click here to see a list of others

The diagram below shows possible interactions between three molecules with dipoles as you can see there are quite a few to consider even with such a small system of molecules

This is why we are using the program you are running for this project. To give us a good idea of whether the molecules you are testing would be anti malarial drugs the program running calculates the forces between the target and your drug. This tells us how tightly the drug would bind to our target, the tighter the binding the better. Obviously this isn't the only test that would need to be done, to read more about how drugs are designed and tested click here.

Hydrophilicity Test

Check your understanding of hydrophilicity below.

Task: You must sort Polar and Non-Polar

Polar	Non-Polar	Sorted
<chem>H-H</chem>	<chem>Cl-H</chem>	<chem>H-F</chem>
<chem>H-N</chem>	<chem>H-C</chem>	<chem>H-O</chem>
<chem>H-O</chem>	<chem>H-C</chem>	<chem>H-C</chem>
<chem>H-C</chem>	<chem>H-C</chem>	<chem>H-C</chem>
<chem>H-C</chem>	<chem>H-C</chem>	<chem>H-C</chem>

Portsmouth outline stadium plan
Cyclists win US endurance race

<http://chemtools.chem.soton.ac.uk/projects/emalaria/>

Open Science Experiment

e @malaria

Home CCDC Lifecycle e-Malaria Project Background Southampton Schools eScience Publications Malaria Introduction Symptoms Treatments Prevention

eCrystals

Home About Browse by Year Browse by People

University of Southampton

N-(4-methylphenyl)acetamide

Sample Originator: Tony L. Threlfall^a.
Data Collection: Susanne L. Huth^a
Structure Determination: Susanne L. Huth^a, Michael B. Hursthouse^a and Simon J. Coles^a
University of Southampton^a
 $C_9H_{11}NO$
 $[\text{InChI}=1\text{C9H11NO}[\text{Oc}1\text{-}7\text{-}5\text{-}6\text{-}4\text{-}7)\text{10\text{-}8}]\text{11h3,6H,1-2H3,(H,10,11)]}$
Identification: 10.3737/eocrystals.chem.soton.ac.uk/544
Number:
Controlled: para-substituted acetanilide
Keywords:
Date: 21 June 2008
Created:
Deposited: 01 Aug 2008 17:29
On:
Deposited By: Ms L.S. Huth
By:
Data collection parameters
Chemical formula: $C_9H_{11}NO$

Available Files

Final Result
 $2008ish008.cif$ 11k
 $2008ish008.cml$ 3k
 $2008ish008.ccf$ 89k

Validation
 $2008ish008_checkcf.htm$ 7k

Insert Molecule

Molecule Name: N-(4-methylphenyl)acetamide

File Edit View Insert Tools Help

H C N O F Root Select Paste Undo Redo Zoom ?

More

Chemical structure: CC(=O)NC1=CC=C(C)C=C1

Molecule N 4 methylphenyl acetamide

CC(=O)NC1=CC=C(C)C=C1

3D

Jobs

Add a Docking Job to target: Malaria DHFR

Id	9213
Name	N 4 methylphenyl acetamide
Smile	<chem>CC(=O)NC1=CC=C(C)C=C1</chem>
InChI	$[\text{InChI}=1\text{C9H11NO}[\text{c1\text{-}7\text{-}3\text{-}5\text{-}6\text{-}4\text{-}7)\text{10\text{-}8}]\text{11h3-6H,1-2H3,(H,10,11)]}$
Status	3D
Jobs	0/0 (0.00:0.00)

Jobs

Add a Docking Job to target: Malaria DHFR

Id	9213
Status	Run Time
H-Bonds	
Wdv	
Strain	
Energy	
Tools	

© University of Southampton 2005
For more information, please email emalaria@soton.ac.uk

Jmol - N 4 methylphenyl acetamide

http://chemtools.chem.soton.ac.uk/projects/emalaria/jmol.php?file=N_4_methylphenyl_acetamide.cif

Molecule N 4 methylphenyl acetamide

CC(=O)NC1=CC=C(C)C=C1

3D

Jobs

Add a Docking Job to target: Malaria DHFR

Id	9213
Name	N 4 methylphenyl acetamide
Smile	<chem>CC(=O)NC1=CC=C(C)C=C1</chem>
InChI	$[\text{InChI}=1\text{C9H11NO}[\text{c1\text{-}7\text{-}3\text{-}5\text{-}6\text{-}4\text{-}7)\text{10\text{-}8}]\text{11h3-6H,1-2H3,(H,10,11)]}$
Status	3D
Jobs	1/1 (37.59:37.59)

Jobs

Add a Docking Job to target: Malaria DHFR

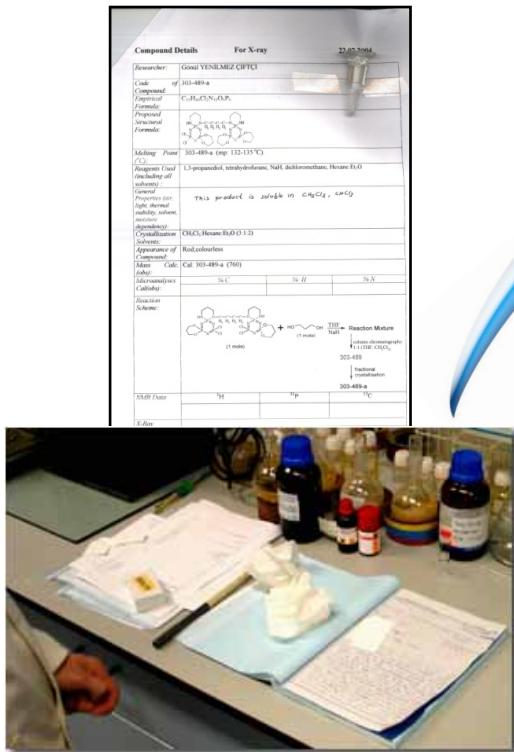
Id	9213
Status	Run Time
H-Bonds	
Wdv	
Strain	
Energy	
Tools	

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For more information, please email emalaria@soton.ac.uk

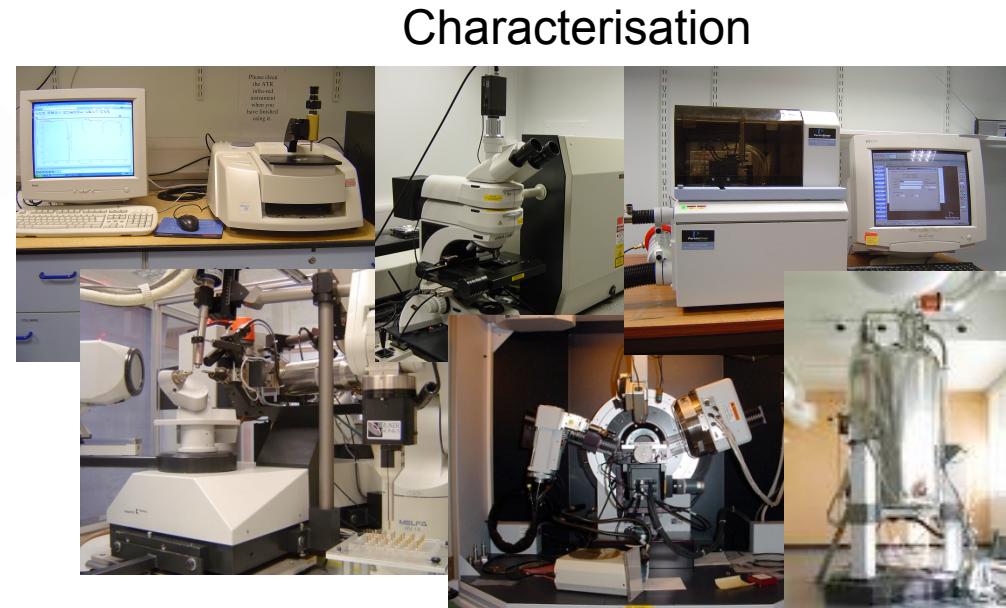
Legend:

- Dark blue: spin
- Green: off
- Pale blue: block
- White background: whiteBackground
- Magenta Drug Molecule: CPK
- Green Top: CPK
- Cyan Right: CPK

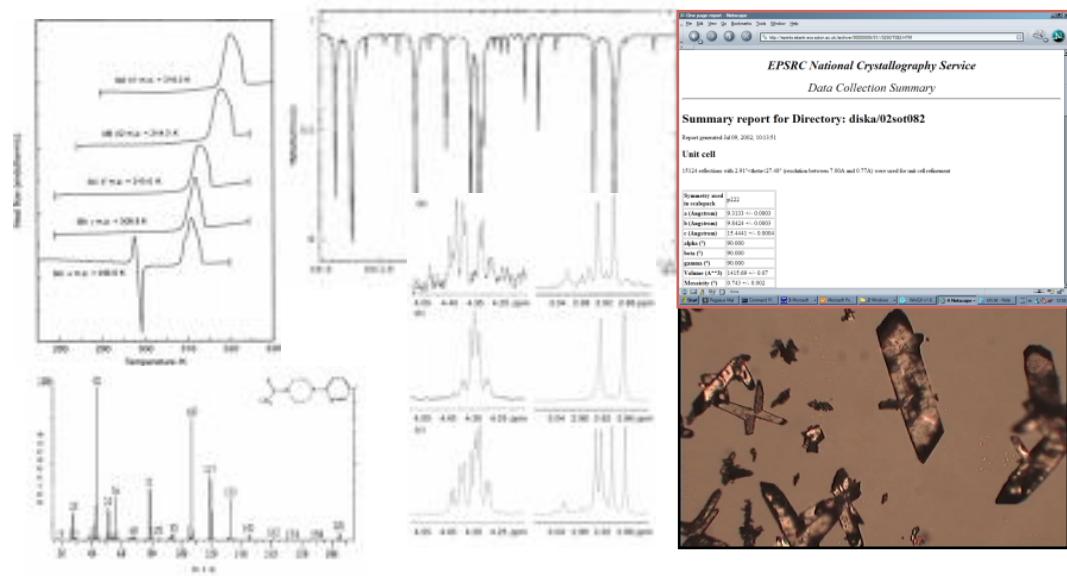
General Chemistry Issues: Data Generation



Synthesis



Characterisation



Shortfalls in Data Management

“Data from experiments conducted as recently as six months ago might be suddenly deemed important, but those researchers may never find those numbers – or if they did might not know what those numbers meant”

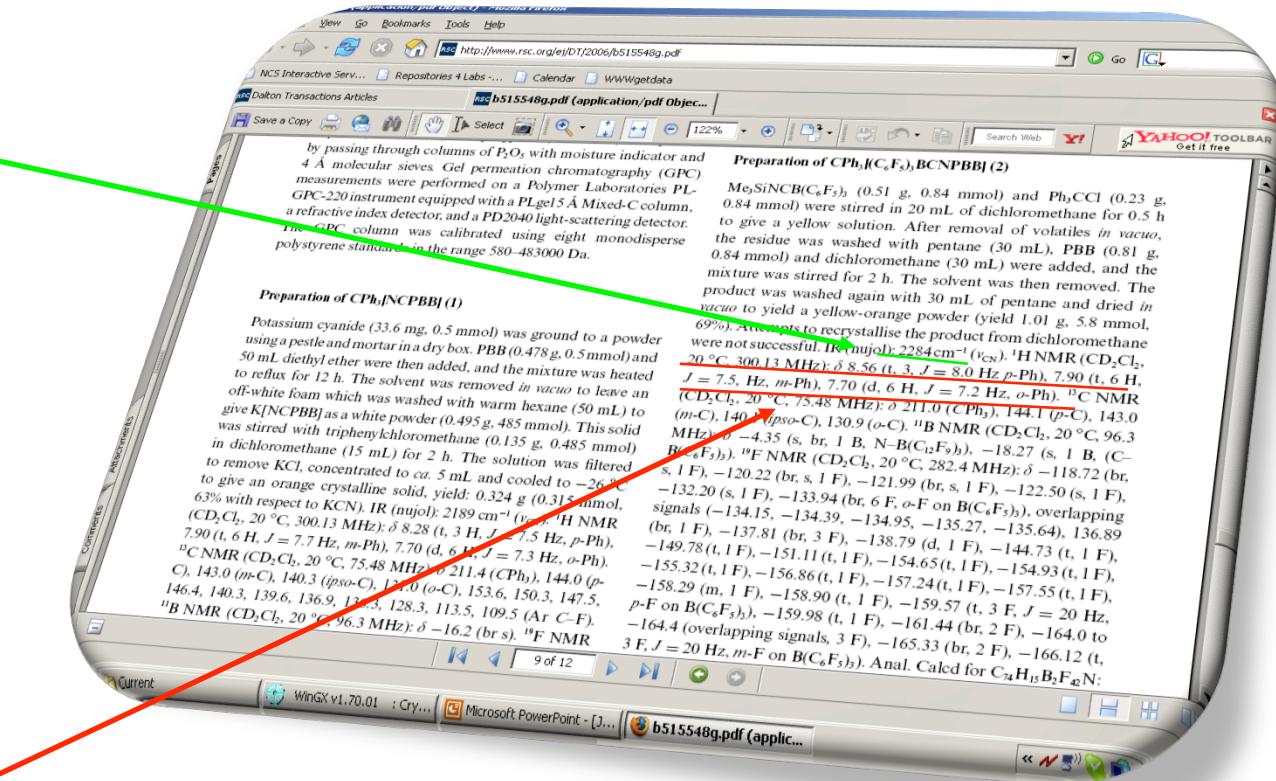
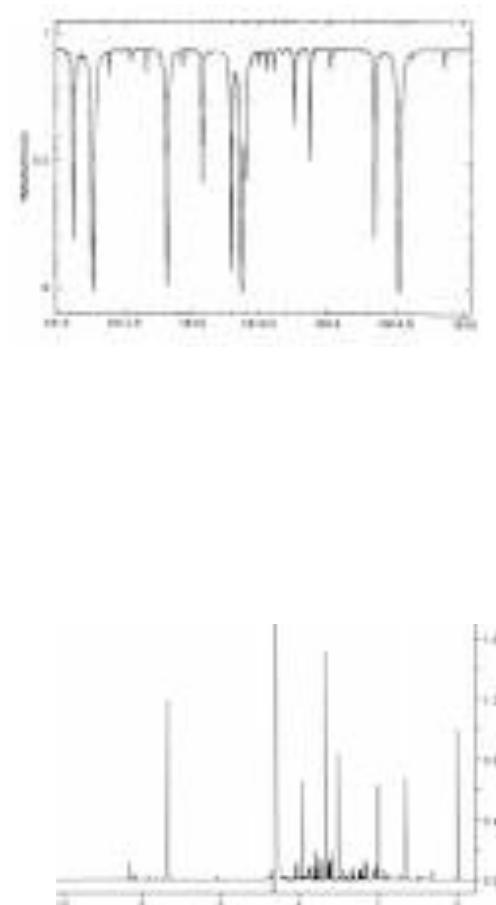
“Lost in some research assistant’s computer, the data are often irretrievable or an undecipherable string of digits”

“To vet experiments, correct errors, or find new breakthroughs, scientists desperately need better ways to store and retrieve research data”

“Data from Big Science is ... easier to handle, understand and archive. Small Science is horribly heterogeneous and far more vast. In time Small Science will generate 2-3 times more data than Big Science.”

‘Lost in a Sea of Science Data’ S.Carlson, The Chronicle of Higher Education (23/06/2006)

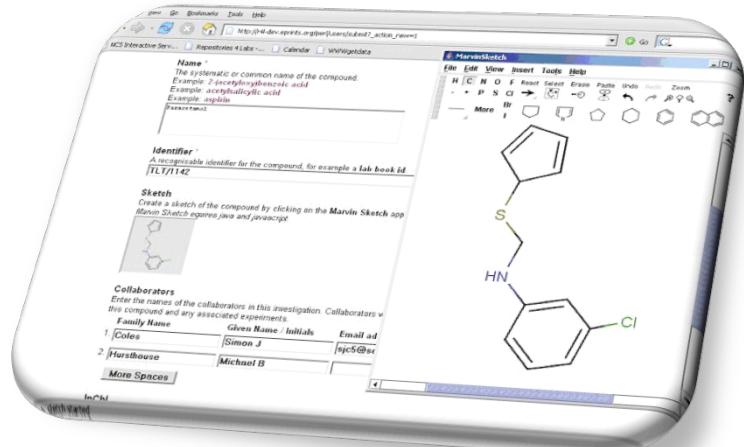
Analysis Data Publication & Information Loss



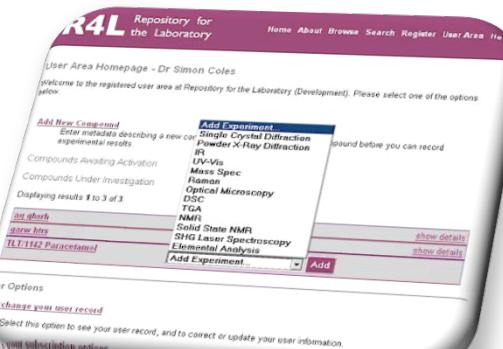
Spectroscopic analysis is often performed to ensure a reaction is proceeding according to plan – as a result <5% are published (via a process with heavy information loss)

A General Chemistry Laboratory Repository

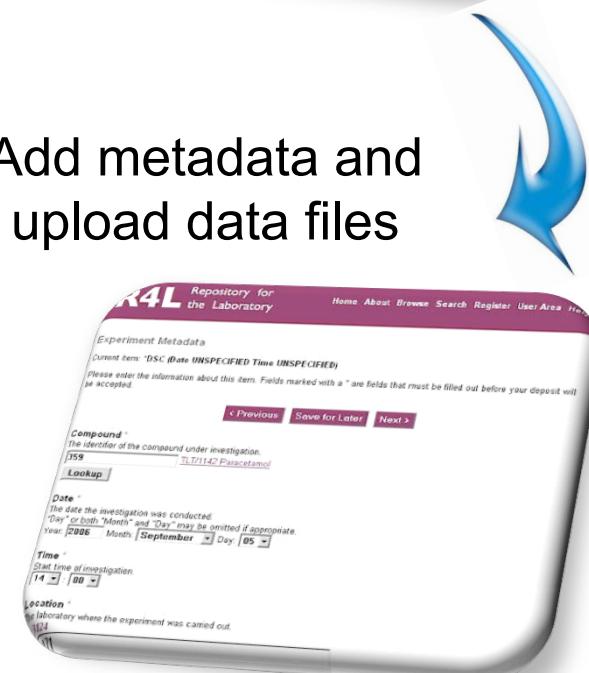
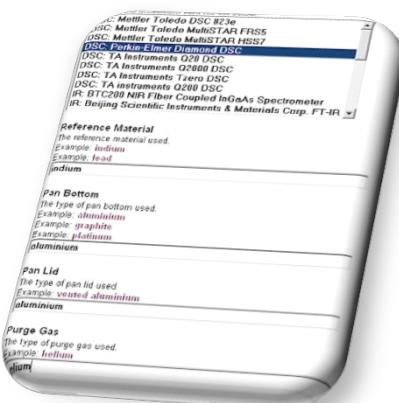
Create new compound
(parent record)



Add new experiment type



Add metadata and
upload data files



Open Science Experiment

R4L Repository for the Laboratory

Home About Browse Search Register User Area Help

DSC Metadata

Current item: *DSC (11 August 2008 16:00)
Please enter the information about this item. Fields marked with a * are fields that must be filled out before your deposit will be accepted.

< Previous Save for Later Next >

Instrument:
Choose an instrument from the list below:
DSC Mettler Toledo DSC 823e
DSC Mettler Toledo MultiSTAR 4155
DSC TA Instruments Q2000 DSC
IR: FT/IR Nicolet Instruments & Materials Corp. FT-IR

Reference Material:
The reference material used.
Example: indium
Example: lead
I

Pan Bottom:
The type of pan bottom used.
Example: aluminum
Example: graphite
Example: platinum

Pan Lid:
The type of pan lid used.
Example: lead

Purge Gas:
The type of purge gas used.
Example: helium

R4L Repository for the Laboratory

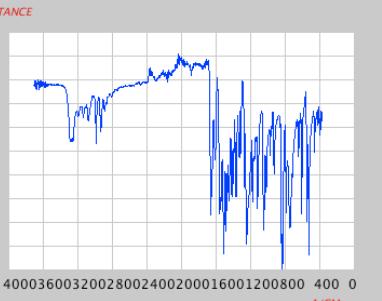
Home About Browse Search Register User Area Help

*IR (08 August 2008 14:10)

- [TLT544-2.JDX \[19 Kb\]](#)
- [TLT544-2.SPA \[9 Kb\]](#)

wdx Spectrum Viewer

TRANSMITTANCE



1.100
1.050
1.000
0.950
0.900
0.850
0.800
0.750
0.700
0.650
0.600

4000 3600 3200 2800 2400 2000 1600 1200 800 400 0

1/cm

TLT544-2

Compound: [TLT544-2 N-\(4-ethoxyphenyl\)acetamide](#)

Location: 30:3067

ID Code: 396

Deposited By: [Dr Simon Coles](#)

Deposited On: 08 August 2008

Contact Information

R4L Repository for the Laboratory

Home About Browse Search Register User Area Help

User Area Homepage - Dr Simon Coles

Welcome to the registered user area at Repository for the Laboratory (Development). Please select one of the options below.

Add New Compound
Enter metadata describing a new compound. You must **activate** the compound before you can record experimental results.

Compounds Awaiting Activation

Compounds Under Investigation

Displaying results 1 to 6 of 6.

ag.ghash	show details	sign off
garw.htrs	show details	sign off
TLT1/142 Paracetamol	show details	sign off
TLT538/2 N-(4-methoxyphenyl)acetamide	show details	sign off
TLT539/3 N-(4-methoxyphenyl)acetamide	show details	sign off
TLT544/2 N-(4-ethoxyphenyl)acetamide	show details	sign off

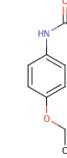
*IR (08 August 2008 14:10)
*DSC (11 August 2008 16:00)
Optical Microscopy (08 August 2008 15:30)

Add Experiment... Add

R4L Repository for the Laboratory

Home About Browse Search Register User Area Help

TLT544/2 N-(4-ethoxyphenyl)acetamide



Collaborators: Coles, Simon J and Huth, Susanne L and Threlfall, Terry L

InChI: InChI=1/C10H13NO2/c1-3-13-10-6-4-9(5-7-10)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)

ID Code: 389

Deposited By: [Dr Simon Coles](#)

Deposited On: 08 August 2008

Experimental Results:

- *IR (08 August 2008 14:10)
- *DSC (11 August 2008 16:00)
- Optical Microscopy (08 August 2008 15:30)

Repository Staff Only: [edit this item](#)

Contact Information

<http://r4l.eprints.org>

A New Kind of Electronic Lab Notebook

moreTea
experiment browser

Sign In

Username
Password
Sign In

Welcome

moreTea is an electronic experiment planning, recording and reviewing tool. It enables you to create experiments, helps you to carry them out, and then lets you view the results and add to your notes.

- 1. Sign Up and Sign In**

Before you can get started using moreTea, you must first create a user profile using the form on the left. You will be sent an e-mail asking you to activate your account. You only have to do this once. If you have already created a profile then just sign in instead.
- 2. Create and Plan**

Once signed in, you can start creating experiments and adding materials and steps to your experiment.
- 3. Record and Observe**

When you've finished planning, it's time to go into the lab and do it for real. The moreTea Lab Tool connects to the server to let you access your experiments in the lab. You can use the Lab Tool to record the amount of each material that you use and make observations by drawing or writing notes.
- 4. Review and Write-up**

Once the experiment is complete you can return to the experiment browser and view the results online. You can also add to the observation notes you made in-lab to expand them as part of your write-up.

Observations/Notes

9.4 g Solid phenol

Draw Write Next step >

© University of Southampton IT Innovation Centre 2007

Add Experiment

Name: N,N'-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarboxamide Identifier: ajb5125/55

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

Add Experiment **Cancel**

My Experiments

You have 28 experiments

Add experiment

Tb Complexation by N,N'-bis(2-aminomethyl)1,8-naphthyridine carboxamide

ajb5125/51 (In Progress)

Small scale test of Tb Complexation by N,N'-bis(2-aminomethyl)1,8-naphthyridine carboxamide

Materials (3 of 4 measured) **Procedure (4 of 5 steps complete)**

m³ m³ ³
O₂ O₂
°C ^C

50.0 mg N,N'-bis-[(2-aminomethyl)pyridine]-1,8-naphthyridine dicarboxamide (50.5 mg used)
23.0 mg Terbium Chloride Hydrate (24.0 mg used)
10.0 mg Sodium Hydroxide
10.0 ml Methanol (12.0 ml used)

Add Step

Add material

Safety

Methanol
Highly Flammable, Toxic, Risk of irreversible effects by all routes

N,N'-bis-[(2-aminomethyl)pyridine]-1,8-naphthyridine dicarboxamide
Treat as toxic

Sodium Hydroxide
Causes Burns

Terbium Chloride Hydrate
Irritating to skin

A New Kind of Electronic Lab Notebook

The diagram illustrates a workflow for a chemical synthesis experiment, showing the integration of various data types and media within a single platform.

Procedure Page: The top-left window shows a detailed procedure for the preparation of *N,N*-bis(pyridin-2-ylmethyl)-1,8-naphthyridine-2,7-dicarboxamide. The "Procedure" section contains 11 steps, with the first step highlighted. The "Materials" and "Safety" sections provide a list of required chemicals and their properties.

Measurement Screen: The top-right window shows the "Measure" tab of the Lab Tool. It lists the materials measured: 1,8-Naphthyridine-2,7-dicarbonyl dichloride, 2-(aminomethyl)pyridine, Dichloromethane, and Triethylamine. The "Status" section indicates 0 of 4 materials have been measured, and 0 of 10 steps have been completed.

Observation Screen: The bottom-right window shows the "Observe" tab. It includes sections for "COSHH Information", "Atomic Weight", and "Required". The "Observations/Notes" section contains a note: "This drew a little more colour off the organic layer and left it slightly cloudy and yellow". A "Draw" button is highlighted.

Photograph: The bottom-left image shows a laboratory setting. A person wearing a white glove is using a stylus to draw on a tablet screen, which displays the notes from the observation screen. The background shows various laboratory glassware and equipment.

Arrows: Blue arrows indicate the flow of data from the procedure page through the measurement and observation screens, and finally to the photograph of the lab setup.

Analysis & Discussion: Blogging Experiments

A repository can...

- Allow one to put, store and get
- Provide search and browse functionality
- **NOT** provide the presentation and discussion functions essential to working up a scientific study

Re: PCR of beta-galactosidase third attempt by Jennifer Hale
14th December 2006 @ 11:10

Unfortunately the purification appears not to have gone well. Though I also can't get any consistency from the figures given by the nano-drop. These are the results I got:

	reading 1	reading 2	reading 3	reading 4	reading 5	reading 6	average
PCR product before*	282.3 ng/ μ L	283.4 ng/ μ L	281.1 ng/ μ L	N/A	N/A	N/A	282.3 ng/ μ L
PCR product after*	7.8 ng/ μ L	12.9 ng/ μ L	17.6 ng/ μ L	85.4 ng/ μ L	22.4 ng/ μ L	12.8 ng/ μ L	?

*Both reactions combined together after PCR

I'm going to do another PCR again. That step is working really well. I'm just not sure what to do about purifying it. The only other thing I can try is eluting in TE buffer rather than water (which it says you can also elute into)

In this purification I used preheated water and followed the instructions closely. Perhaps the DNA will elute into TE more effectively.

Re: PCR of beta-galactosidase third attempt by David Neylon
14th December 2006 @ 18:32

I would definitely compare these on a gel so as to see whether it is just the nanodrop that is the problem. It might help also if you are explicit about how much solution you are trying to purify and what the final volume is.

Jennifer Hale / beta-galactosidase preparation and assays | Comments (1)

Comments

Re: Transformation of ligation product jrh4712/86 into competent and supercompetent XL1 Blue by Jennifer Hale
18th January 2007 @ 14:50

A fuller description of each plate can be found by clicking on the image. Left to right through images: competent cell transformations; supercompetent cell transformations; 4 °C vs 14 °C ligations in transformation results, both sets of cells; +ve and -ve controls, both sets of cells.

Sample Parent

jrh4712-74 (1)
jrh4712-76 (1)
jrh4712-76a (1)
jrh4712-77 (1)
jrh4712-79 (1)
jrh4712-80_white (1)
jrh4712-82 (1)
jrh4712-86 (2)
4712-86 (1)
4712-84_beta-gal (1)
4712-80_blue (1)
4712-88 (1)

Product

jrh4712-74 (1)
jrh4712-76 (1)
jrh4712-76a (1)
jrh4712-77 (1)
jrh4712-79 (1)
jrh4712-80_white (1)
jrh4712-82 (1)
jrh4712-86 (2)
4712-86 (1)
4712-84_beta-gal (1)
4712-80_blue (1)
4712-88 (1)

Investigations into neutral drift

Test PCR (different primer, dNTP and enzyme stocks)

post Type PCR risk assessment

reaction	DNA template	ul Water	ul Buffer	ul Primer 1	ul Primer 2	ul dNTPs	ul Miscellaneous	ul Enzyme	ul	Product
1	Purified plasmid from the X-gal positive colonies (025/46 experiment round 4)	Sterile filtered	8.8 GoTaq (04/08)	4 beta-glu fwd	1 Beta-glu rev	1 Normal made 04/08	2 MgCl ₂	1.2 GoTaq (04/08)	1 (diluted 1 in 50)	Test different PCR primer, dNTP and enzyme product 1
2	Purified plasmid from the X-gal positive colonies (025/46 experiment round 4)	Sterile filtered	8.8 GoTaq (04/08)	4 beta-glu fwd 04/08	1 Beta-glu rev 04/08	1 Normal made 04/08	2 MgCl ₂	1.2 GoTaq (04/08)	1 (diluted 1 in 50)	Test different PCR primer, dNTP and enzyme product 2
3	Purified plasmid from the X-gal positive colonies (025/46 experiment round 4)	Sterile filtered	8.8 GoTaq (04/08)	4 beta-glu fwd 13.05.08	1 beta-glu rev 13.05.08	1 Normal made 04/08	2 MgCl ₂	1.2 GoTaq (04/08)	1 (diluted 1 in 50)	Test different PCR primer, dNTP and enzyme product 3
4	None	Sterile filtered	9.8 GoTaq (04/08)	4 beta-glu fwd 13.05.08	1 beta-glu rev 13.05.08	1 Normal made 04/08	2 MgCl ₂	1.2 GoTaq (04/08)	1 (diluted 1 in 50)	Test different PCR primer, dNTP and enzyme product 4

Sections

Notes (71)
Tools (1)
Procedure (38)
Method (127)
Safety (13)
Template (29)

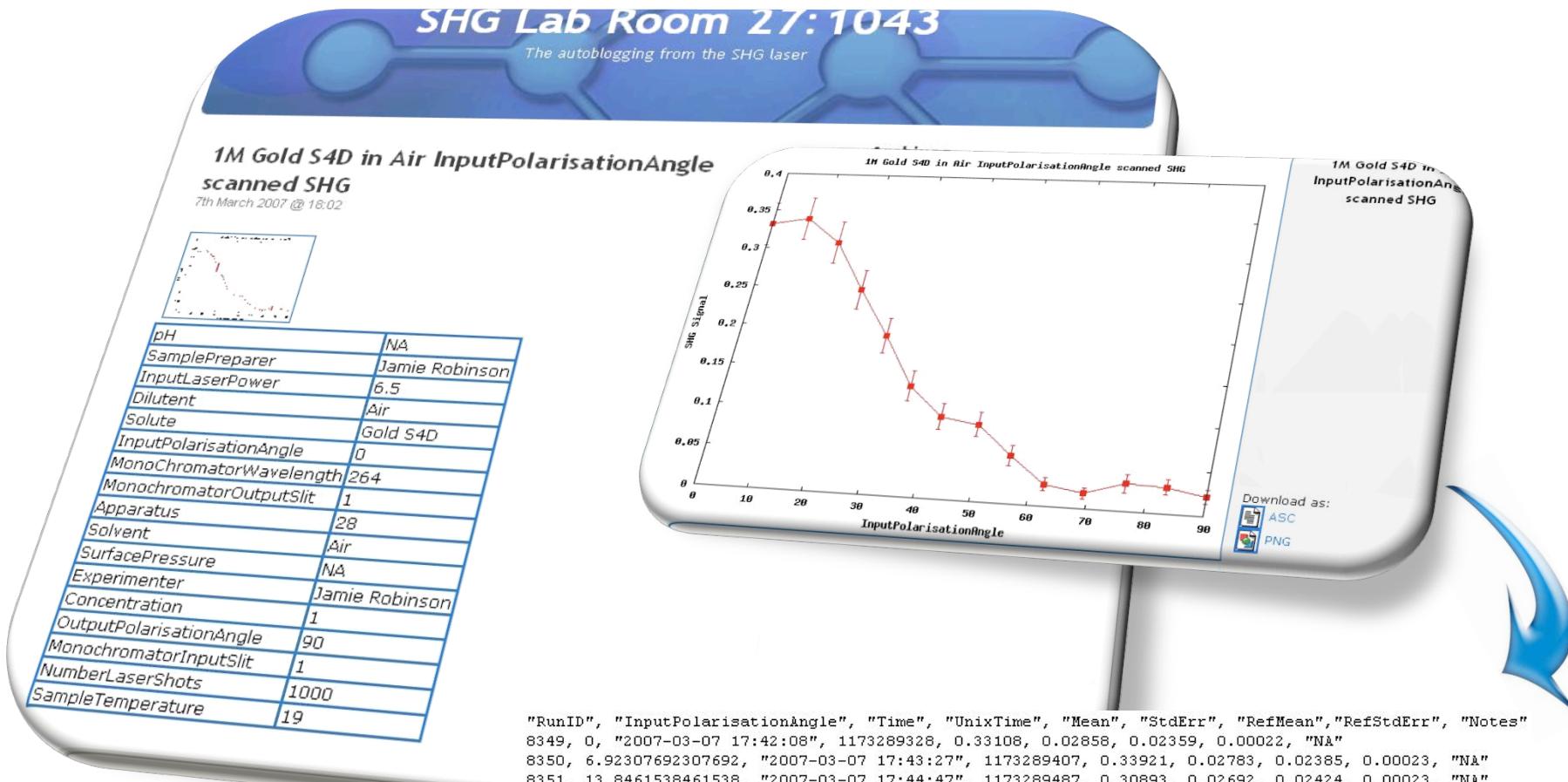
Post Type

Discussion (31)
Experiment (15)
Cat stain (28)
Buffer (38)
Idea (11)
Thermocycle (5)
Template (21)

- Enables 'geographically distributed collaborative research'
- Can be open or private
- A useful approach for sharing 'failed' experiments?

<http://chemtools.chem.soton.ac.uk/projects/blog/>

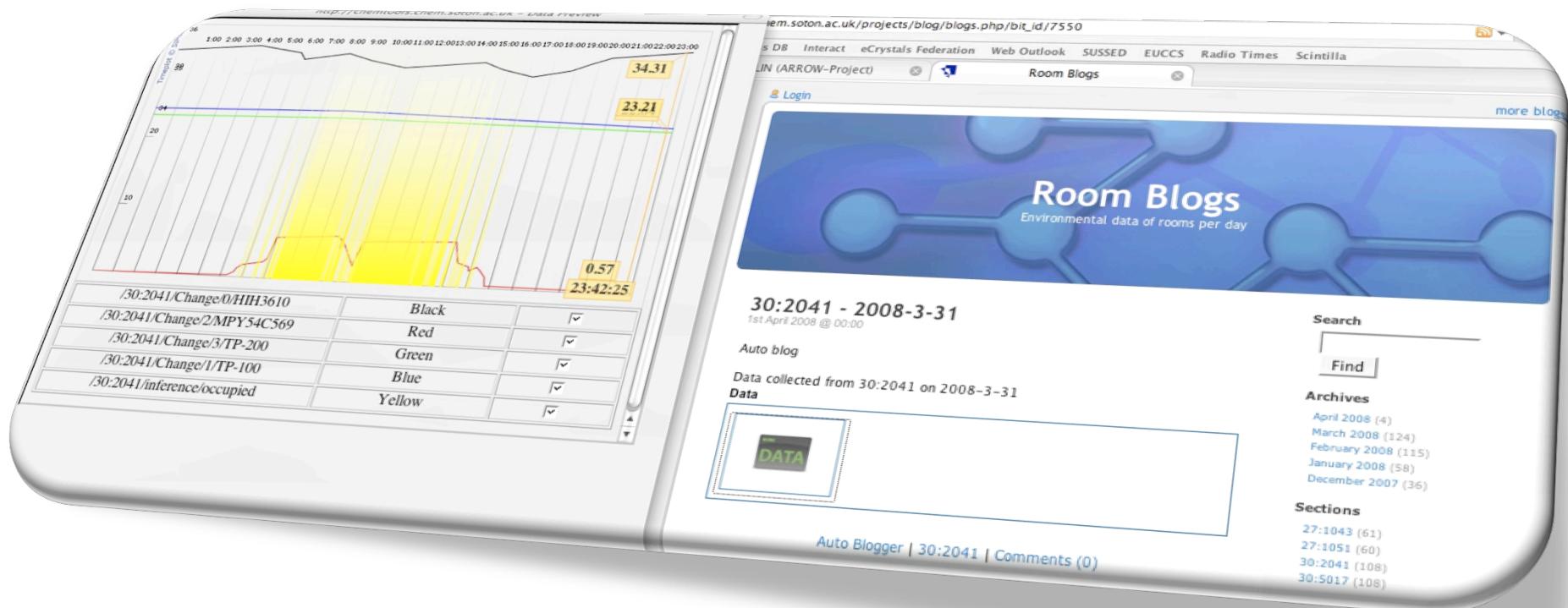
Automatic Blogging by Machines



```
"RunID", "InputPolarisationAngle", "Time", "UnixTime", "Mean", "StdErr", "RefMean", "RefStdErr", "Notes"  
8349, 0, "2007-03-07 17:42:08", 1173289328, 0.33108, 0.02858, 0.02359, 0.00022, "NA"  
8350, 6.92307692307692, "2007-03-07 17:43:27", 1173289407, 0.33921, 0.02783, 0.02385, 0.00023, "NA"  
8351, 13.8461538461538, "2007-03-07 17:44:47", 1173289487, 0.30893, 0.02692, 0.02424, 0.00023, "NA"  
8352, 20.7692307692307, "2007-03-07 17:46:06", 1173289566, 0.24921, 0.02485, 0.02396, 0.00023, "NA"  
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8354, 34.6153846153845, "2007-03-07 17:48:45", 1173289725, 0.13147, 0.01842, 0.02377, 0.00022, "NA"  
8355, 41.5384615384614, "2007-03-07 17:50:05", 1173289805, 0.09684, 0.01536, 0.02407, 0.00023, "NA"  
8356, 48.4615384615383, "2007-03-07 17:51:24", 1173289884, 0.08984, 0.01470, 0.02406, 0.00023, "NA"  
8357, 55.3846153846152, "2007-03-07 17:52:43", 1173289963, 0.05578, 0.01183, 0.02456, 0.00023, "NA"  
8358, 62.3076923076921, "2007-03-07 17:54:03", 1173290043, 0.02520, 0.00770, 0.02401, 0.00023, "NA"  
8359, 69.230769230769, "2007-03-07 17:55:22", 1173290122, 0.01750, 0.00661, 0.02438, 0.00023, "NA"  
8360, 76.1538461538459, "2007-03-07 17:56:41", 1173290201, 0.03136, 0.00998, 0.02397, 0.00023, "NA"  
8361, 83.0769230769228, "2007-03-07 17:58:01", 1173290281, 0.03012, 0.00846, 0.02393, 0.00023, "NA"  
8362, 89.9999999999997, "2007-03-07 17:59:20", 1173290360, 0.02174, 0.00789, 0.02383, 0.00023, "NA"
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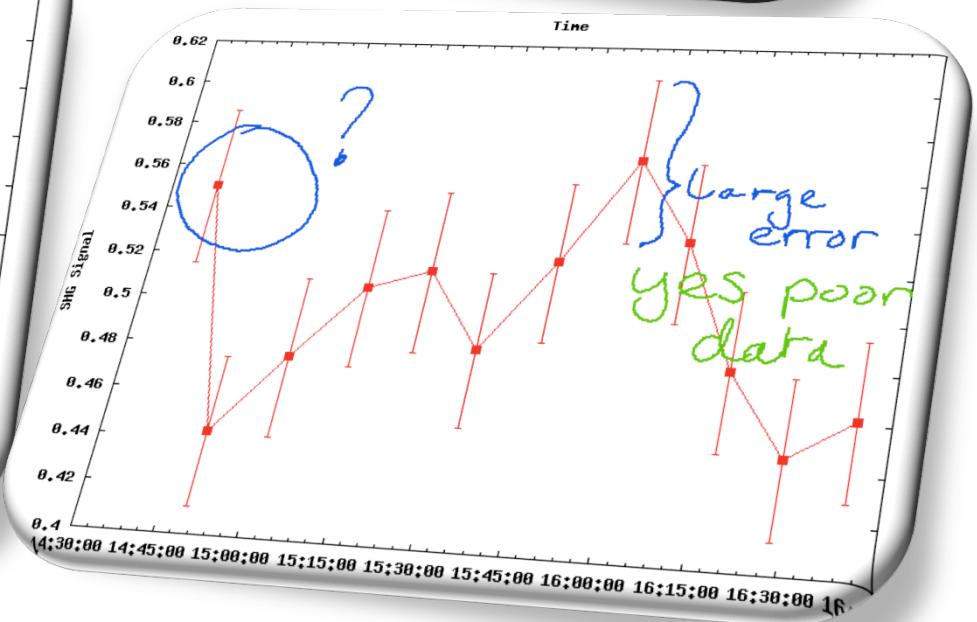
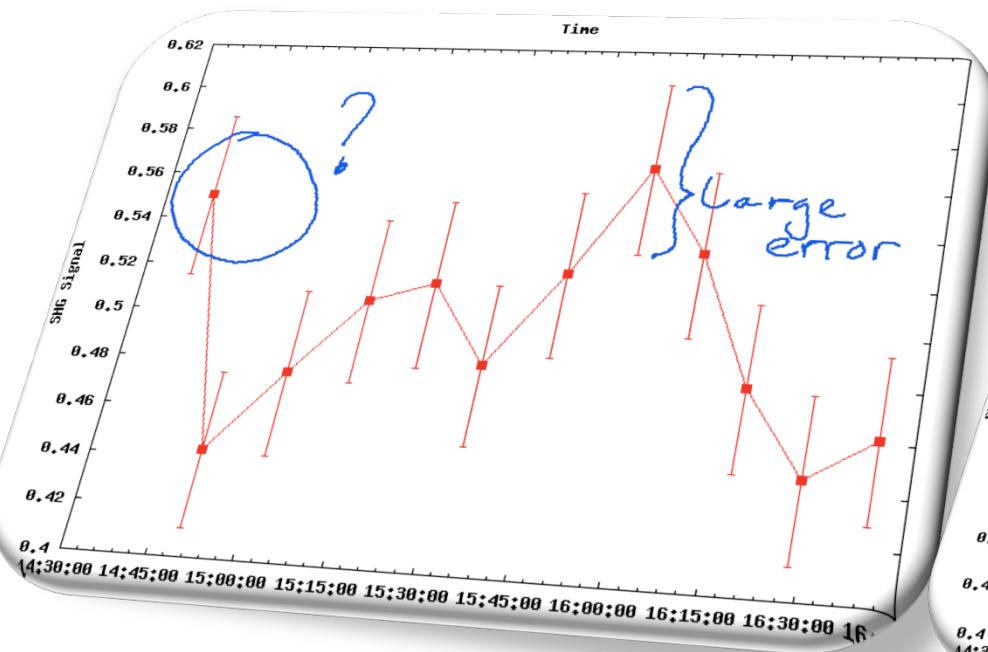
Automatic Blogging by Sensors

- Continuous log of 'environmental' conditions in a laboratory
- Instant detection of erroneous events
- Correlate with inconsistencies in datasets



Comments and Collaborative Tools

- Annotation tools allow comments and foster collaboration and / or communication
- Need for more advanced Blog tools / technology around data



Open Science Experiment

eCrystals

Edit Post

Title: N-(4-methoxyphenyl)acetamide HSM

Text: <http://r4i-dev.eprints.org/395/>

Deposited at: <http://r4i-dev.eprints.org/395/>

Groups: Structural Systematics and Structure-Property (2)

Metadata: key: Creators value: Simon_Coles

key: Experiment Type value: Hot_Stage_Microscopy

Reason For Edit: [Submit](#) [Preview](#)

Live Copy

[Copy In](#) or upload data



N-(4-methoxyphenyl)acetamide HSM

18th August 2008 @ 13:02

Creators: Simon_Coles

Experiment Type: Hot_Stage_Microscopy

Deposited at: <http://r4i-dev.eprints.org/395/>

Acetylation of amines – general synthetic route

N-(4-methoxyphenyl)acetamide DSC

19th August 2008 @ 12:59

Creators: Simon_Coles

Experiment Type: DSC

DSC deposited at: <http://r4i-dev.eprints.org/399/>

Acetylation of amines – general synthetic route

Fast rate = 100degrees/min
Slow rate = 10degrees/min

[Simon_Coles](#) | [Edit Post](#) | [Structural Systematics and Structure-Property](#) | [Comments \(0\)](#)

Acetamide project eMalaria docking results

18th August 2008 @ 16:18

Creators: Simon_Coles

Experiment Type: eMalaria_docking_job

Total energy = 37.59, 37.01, 41.74 kJ mol⁻¹ for Me, OMe, OEt respectively

Broken down to:

Me = 5.53, 26.87, -4.89
OMe = 5.41, 27.57, -6.31
OEt = 5.76, 31.44, -7.26

for h-bond, Van Der Waals and Strain contributions respectively.

This reflects the greater degree of freedom in the OEt chain, whereas OMe and Me are relatively similar.

Acetylation of amines - general synthetic route

N-(4-methoxyphenyl)acetamide crystal structure N-(4-methoxyphenyl)acetamide

methylphenylacetamide crystal structure N-(4-ethoxyphenyl)acetamide

crystal structure N-(4-ethoxyphenyl)acetamide

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Acetylation of amines - general synthetic route

19th August 2008 @ 12:22

Creators: Terry_Threlfall

Experiment Type: Synthesis

There are several reagents and procedures which can be used to convert an aromatic amine to an acetanilide. For example, the practical textbooks describe heating an aromatic amine with acetic anhydride, preferably in the presence of a trace of mineral acid and distilling off the acetanilide that forms. However this will only work if the amine has a convenient benzene ring substituent, i.e. fairly reactive. More reactive reagents and more convenient for small-scale use are acetic anhydride and acetyl chloride. For poorly reactive (feebly basic) amines, acetyl bromide is often used. Large numbers of substituted amines were being acylated in the present series of experiments from which these three examples were taken, and so it was desirable to have a general procedure. Some of the amines were relatively insoluble in solvents, so water was used as the solvent. Acetyl chloride was chosen as the acylation agent. Pyridine was used as the solvent because it is a powerful solvent which catalyses the acylation process. However, acetyl chloride and pyridine react vigorously together. So the following procedure was adopted. The solid which formed was filtered off and recrystallised from ethanol. Ethanol is generally the most effective solvent for the formation of crystals of amides, suitable for single crystal x-ray diffraction studies. Some amides are rather too soluble and aqueous ethanol or hydrocarbon solvents may then be more appropriate. The above procedure is vigorous and so is suitable only for the small scale used here.

This Post is Linked By: N-(4-methoxyphenyl)acetamide; N-(4-methoxyphenyl)acetamide Crystal Structure; N-(4-methoxyphenyl)acetamide Infra-Red; N-(4-methoxyphenyl)acetamide DSC; N-(4-methoxyphenyl)acetamide crystal structure; Acetamide project eMalaria docking results; N-(4-ethoxyphenyl)acetamide HSM; N-(4-methoxyphenyl)acetamide Hot Stage Microscopy; N-(4-methoxyphenyl)acetamide Infra-Red;

eCrystals

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New Post

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August 2008 (13)

July 2008 (3)

Sections

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Structural Systematics and Structure-Property (13)

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Simon_Coles, Ryan_Warnock (1)

Terry_Threlfall (1)

Simon_Coles (12)

Experiment Type

Synthesis (1)

Infra-Red (3)

Crystal Structure (3)

Hot_Stage_Microscopy (2)

DSC (1)

Misc

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Open Science Experiment

The screenshot shows a web page from the eCrystals platform. The header features the 'eCrystals' logo with a blue molecular structure background. The main content is a discussion post titled 'Acetanilide comparison' by 'Simon_Coles' on 18th August 2008 at 17:42. The post discusses the comparison of N-(4-methylphenyl)acetamide, N-(4-methoxyphenyl)acetamide, and N-(4-ethoxyphenyl)acetamide. It mentions that the OMe derivative might contain some water, but this is not present in the crystal structure. The DSC analysis shows no unusual behaviour, with melting points of 117, 135 degreesC for Me, OMe & OEt respectively. The post concludes with a note about crystal packing and spatial separation. The sidebar includes a search bar, links for 'Admin' and 'New Post', and sections for 'Archives' (August 2008, July 2008), 'Sections' (Development, Structural Systematics and Structure-Property), 'Creators' (Simon_Coles, Ryan_Warnock, Terry_Threlfall, Simon_Coles), and 'Experiment Type' (Synthesis, Infra-Red, Crystal_Structure, DSC, eMalaria_docking_job, Hot_Stage_Microscopy, Discussion).

eCrystals

Acetanilide comparison
18th August 2008 @ 17:42

Creators: Simon_Coles
Experiment Type: Discussion

There are few differences in the IR's *N*-(4-methylphenyl)acetamide/*N*-(4-methoxyphenyl)acetamide Infra Red/*N*-(4-ethoxyphenyl)acetamide Infra-Red - the OMe derivative might contain some water, however this is not present in the crystal structure *N*-(4-methoxyphenyl)acetamide crystal structure? DSC *N*-(4-methoxyphenyl)acetamide DSCN-(4-ethoxyphenyl)acetamide DSCN-(4-methylphenyl)acetamide DSC shows no unusual behaviour in any of the compounds and melting points agree with hot stage microscopy (145, 117, 135 degreesC for Me, OMe & OEt respectively) *N*-(4-methoxyphenyl)acetamide Hot Stage Microscopy *N*-(4-methoxyphenyl)acetamide HSMN-(4-methylphenyl)acetamide Hot Stage Microscopy. Reason for melting point difference in OMe compound appears to be result of crystal packing: the crystal structures *N*-(4-ethoxyphenyl)acetamide crystal structure *N*-(4-methoxyphenyl)acetamide crystal structure *N*-(4-methylphenyl)acetamide Crystal Structure exhibit the same strong intermolecular hydrogen bonds and similar packing motifs, however OMe spatial separation appears to be different...an XPac analysis is required.

[Simon Coles](#) | [Edit Post](#) | [Structural Systematics and Structure-Property](#) | [Comments \(0\)](#)

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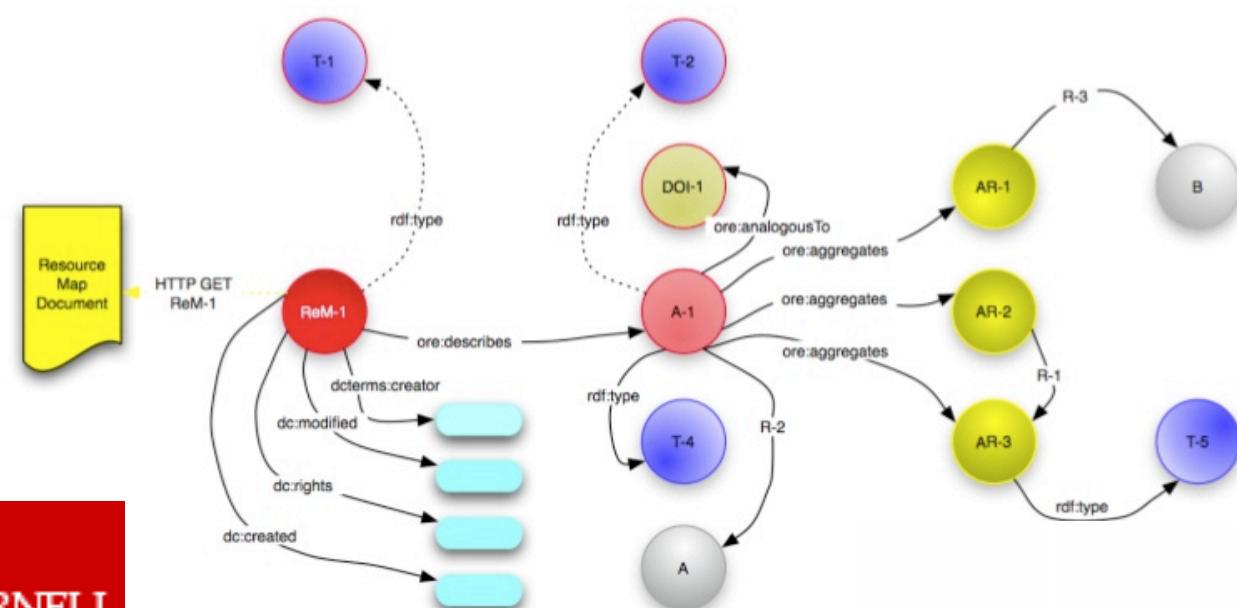
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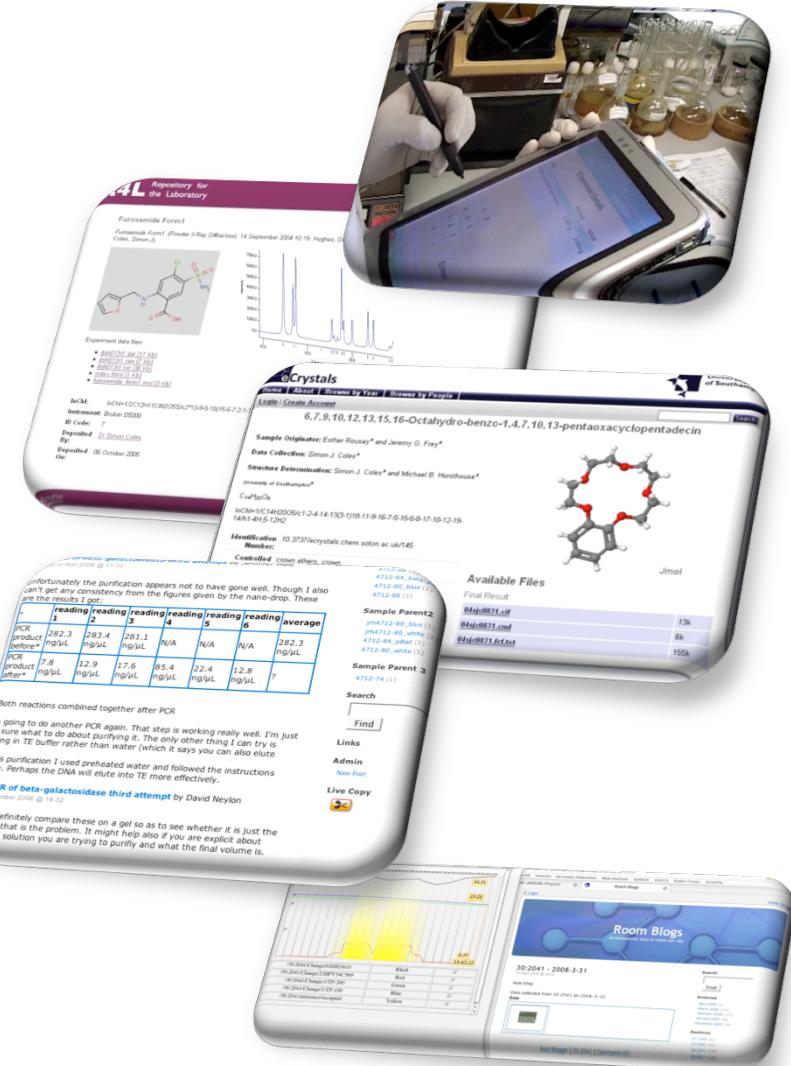
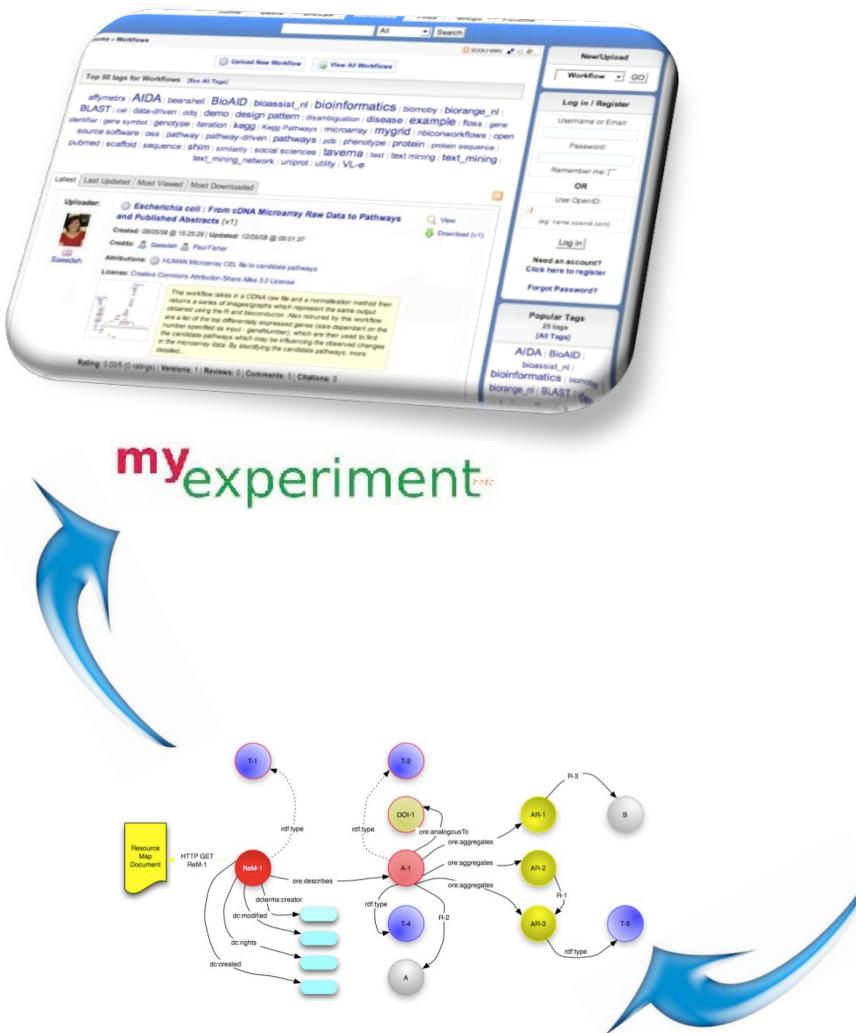
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[Hot_Stage_Microscopy \(3\)](#)
[Discussion \(1\)](#)

Packaging, Describing and Sharing

- New moves in Digital Libraries community to enable distributed repositories to exchange content
- OAI-ORE (Open Archives Initiative – Object Reuse and Exchange)
- <http://www.openarchives.org/ore/>
- Describes an aggregation of objects in an exchangeable format
- Microsoft funded eChemistry testbed project



Towards a New Model for Chemical Information Exchange



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Site Announcements

myExperiment design paper published 07/08/08 @ 12:05:32 by David De Roure

Significant changes to Biomart filters and attributes! Please check your workflows! 04/08/08 @ 15:48:55 by Franck Tanoh

myExperiment has 1000 registered users 28/07/08 @ 15:26:02 by David De Roure

New myExperiment and WHIP plugin for Taverna 28/07/08 @ 15:07:55 by Jiten Bhagat

wiki.myexperiment.org new and improved for developers 28/07/08 @ 15:02:03 by David De Roure

My News

No news

Updated Items

File: Article List Viewer Blocks by Jiro (13 hours ago)
File: Genbank Cross Reference Blocks by Jiro (14 hours ago)
Pack: Provenance challenge by Paul Fisher (6 days ago)
File: A Test of myExperiment's file uploading by Yiming Sun (11 days ago)
File: An Introduction to Taverna and myExperiment - Background by Paul Fisher (13 days ago)
File: A Taverna Users Guide by Paul Fisher (14 days ago)
Pack: Newcastle NeuroScience by Paul Fisher (14 days ago)
Workflow: Perform a text based search through PubMed by Paul Fisher (16 days ago)
File: random workers ages data by Ptimus (16 days ago)

New/Upload

Workflow

 Simon Coles

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2 friends | 0 groups | 1 Blogs | 2 Files

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Open Science Experiment

Home > Packs > acetanilide comparison study (test)

All Search

Item successfully added to pack.

[Manage Pack](#) [Delete Pack](#)

Pack: acetanilide comparison study (test)

Created at: 18/08/08 @ 17:58:31 Last updated: 18/08/08 @ 17:58:31

[Add item] [Sharing] [Tags (5)] [Featured in Packs (0)] [Favoured By (0)] [Comments (0)]

Title: acetanilide comparison study (test)

Description

Links to repository records, data files and Blog discussions for infra-red, hot stage microscopy, differential scanning calorimetry and x-ray crystallography studies on a small family of simple acetanilides

[edit]

Items (1)

External: Link - (<http://ecrystals.chem.soton.ac.uk/544>)  

[Add a comment here] Added by Simon Coles ... less than a minute ago (18/08/08 @ 17:59:57)

Add an Item

Quick add: (a link) eg: "http://www.myexperiment.org/workflows/1" or "http://www.example.com/something-nice" [Add](#)

IR, DSC, HSM
Added by Simon Coles ... 1 minute ago (18/08/08 @ 18:09:50)

External: N-(4-methylphenyl)acetamide data - (<http://4i-dev.eprints.org/390>)  

IR, DSC, HSM
Added by Simon Coles ... 2 minutes ago (18/08/08 @ 18:08:32)

External: Blog discussion & comparison - (http://chemtools.chem.soton.ac.uk/projects/blog/blogs.php?blogs.php!31/meta/EXPERIMENT_TYPE!value/Discussion)  

[Add a comment here] Added by Simon Coles ... 6 minutes ago (18/08/08 @ 18:04:56)

External: OET crystal structure - (<http://ecrystals.chem.soton.ac.uk/547>)  

[Add a comment here] Added by Simon Coles ... 8 minutes ago (18/08/08 @ 18:02:26)

External: OME crystal structure - (<http://ecrystals.chem.soton.ac.uk/543>)  

[Add a comment here] Added by Simon Coles ... 9 minutes ago (18/08/08 @ 18:01:38)

External: Me crystal structure - (<http://ecrystals.chem.soton.ac.uk/544>)  

[Add a comment here] Added by Simon Coles ... 11 minutes ago (18/08/08 @ 17:59:57)

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 Simon Coles

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1 item in this pack

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acetanilide | crystal structure | differential scanning calorimetry | hot stage microscopy | infra-red spectroscopy

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Creator:

 Simon Coles

acetanilide comparison study (test)

Created: 18/08/08 @ 17:58:31 | Updated: 18/08/08 @ 17:58:31

Links to repository records, data files and Blog discussions for infra-red, hot stage microscopy, differential scanning calorimetry and x-ray crystallography studies on a small family of simple acetanilides

7 items in this pack

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acetanilide | crystal structure | differential scanning calorimetry | hot stage microscopy | infra-red spectroscopy

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1 Blogs 1 Packs 2 Files 2 Favourites

Simon Coles has been credited 0 times

Simon Coles has an average rating of: 0.0 / 5

(0 ratings in total) for their items

Name: Simon Coles [edit](#)

Joined: Wednesday 07 November 2007 @ 16:05:59 (GMT)

Last seen: Monday 18 August 2008 @ 17:45:25 (BST)

Email (public): s.j.coles [at] soton.ac.uk

Website: Not specified

Location: Southampton, United Kingdom

Note: the information here is private and cannot be seen by anyone else.

Username: sjc5

Openid url: <http://sjcoles.myopenid.com/>

Account Email: s.j.coles@soton.ac.uk

Description/summary not set

Other contact details:

Field/Industry: Chemistry Academic Research

Occupation/Role(s): Academic

Organisation(s):

University of Southampton

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 Simon Coles

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6 tags

acetanilide | benzene | 15-crown-5 | crystal structure | differential scanning calorimetry | hot stage microscopy | infra-red spectroscopy

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A solid foundation for Open/Self-Publishing and Communication of Chemistry Data???

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- **Liz Lyon, Rachel Heery, Monica Duke, Michael Day, Traugott Koch, Manjula Patel, Pete Cliff**

