

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

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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.tvtoe.com/tvtome/servlet/GuidePageServlet/showid-146/epid-346864/>

Social Networks for Chemists



Google generation: new behaviour and approach

Sharing Rich Media

The image displays three overlapping screenshots of scientific websites, illustrating the integration of video and text in research communication.

Top Screenshot (SciVEE): The SciVEE website (beta) features a navigation bar with 'browse', 'upload', and 'community' buttons. Below the bar, a video player shows a laboratory setting with a person in blue gloves. The video title is 'UCSD Organic Lab: Recrystallization'. To the right of the video, there is a 'Submitted by' field (Joshua Krohn), a 'Description' field (For further details about UCSD Professor Haim Weizman's organic lab and classes please visit: http://chem-courses.ucsd.edu/CoursePages/Uglabs/143A_Weizman/), and a 'Rating' field (5 stars).

Middle Screenshot (JoVE): The JoVE website (JOURNAL OF VISUALIZED EXPERIMENTS) features a navigation bar with 'Welcome', 'About JoVE', 'Editorial Board', 'Press', 'Advertising', 'The Team', and 'Contact Us' buttons. Below the bar, a video player shows a person in a purple shirt. The video title is 'Generation of Stable Transgenic C. elegans Using Microinjection'. To the right of the video, there is a 'Submitted by' field (Laura A. Berkowitz, Adam L. Knight, Guy A. Caldwell, Kim A. Caldwell), a 'Description' field (This video demonstrates the technique of microinjection into the gonad of C. elegans to create transgenic animals.), and a 'Rating' field (5 stars).

Bottom Screenshot (Journal of Visualized Experiments): The Journal of Visualized Experiments website features a navigation bar with 'Subscribe', 'Browse Issues', and 'Categories' buttons. Below the bar, a video player shows a white mouse. The video title is 'Imaging Effector Memory T cells in the Ear After Induction of Adoptive DTH'. To the right of the video, there is a 'Submitted by' field (Melanie P. Mathew¹, Christine Beeton¹, Ian Parker², K. George Chandy¹, Michael D. Cahalan¹), a 'Description' field (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.), and a 'Rating' field (5 stars).

- Video + Paper = Pubcast

New Approaches to 'Sharing Experiments'



- Specialised domain-oriented innovations

Formation of Open Communities



- New approaches surfacing and growing FAST

Open Notebook Science

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

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Navigation: Join this Space, Recent Changes, Manage Space, Search, All Experiments, Mailing List, Docking Libraries, References, Experiment Format, Extra Credit, Paper01 Draft, Paper02 Draft, Isolated Compounds, Alicia's Masters Thesis, CombiUgi Project, To Do List

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

Procedure
A solution of [adrenaline](#) (1.0g 5.5mmoles) in 85% phosphoric acid was heated (110°C) 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 removed by evaporation to give DOPAL (80 mg 0.53mmol, 9.5% yield)

Characterization:
Results
1. [TLC of 25A in 3:1 MeCl₂/ MeOH](#) and in [6:1 MeCl₂/ MeOH](#), and [stained with CAM](#)
2. [HNMR of 25A](#) in acetone-d₆, and the expansions of the prominent peak regions ([one](#) and [two](#))
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 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](#)). The atmosphere should have prevented.

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

My 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 on a mac). I've posted a [simple example electronic lab notebook in latex](#) with the commands and functions that I frequently use. [sample.tex](#) is the main file; see this file to determine if you need to install any of the commands or functions that I use. [sample.pdf](#) is the compiled document. If you don't have latex installed, you can use [this](#) to install it.

Open Science Isn't
Finally, I just want to

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

SATURDAY, JANUARY 19, 2008

New microarray data

The post-docs have finished the first-pass analysis of how *E. coli* gene expression is affected by both the *E. coli* Sxy and the *H. influenzae* Sxy proteins. I suppose I shouldn't be surprised that it's more complicated than I had hoped. For example, unlike the situation in *H. influenzae*, in *E. coli* there are also groups of genes whose expression goes down when Sxy is present.

One complication is that these cells are probably seriously OVER-producing Sxy. Unlike *H. influenzae*, where we've only done arrays of cells expressing a single-copy sxy gene under its natural promoter, these *E. coli* studies used a sxy gene on a high-copy plasmid and under a highly inducible promoter. We know that prolonged expression of Sxy from this plasmid produces large quantities of denatured Sxy (in inclusion bodies) and we don't know the extent to which even the 30-minute expression used for the arrays studies might create a situation unlike that of natural sxy expression.

POSTED BY ROSIE REDFIELD AT 6:25 PM

2 COMMENTS:
playork said...
remember what you've said about sxy in the past. Can you make a null version of

ABOUT ME
ROSIE REDFIELD CANADA
I run a microbiology research lab in the Life Sciences Centre at the University of British Columbia.
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[Data on E. coli protein](#)

- Immediate sharing of experimental information & data

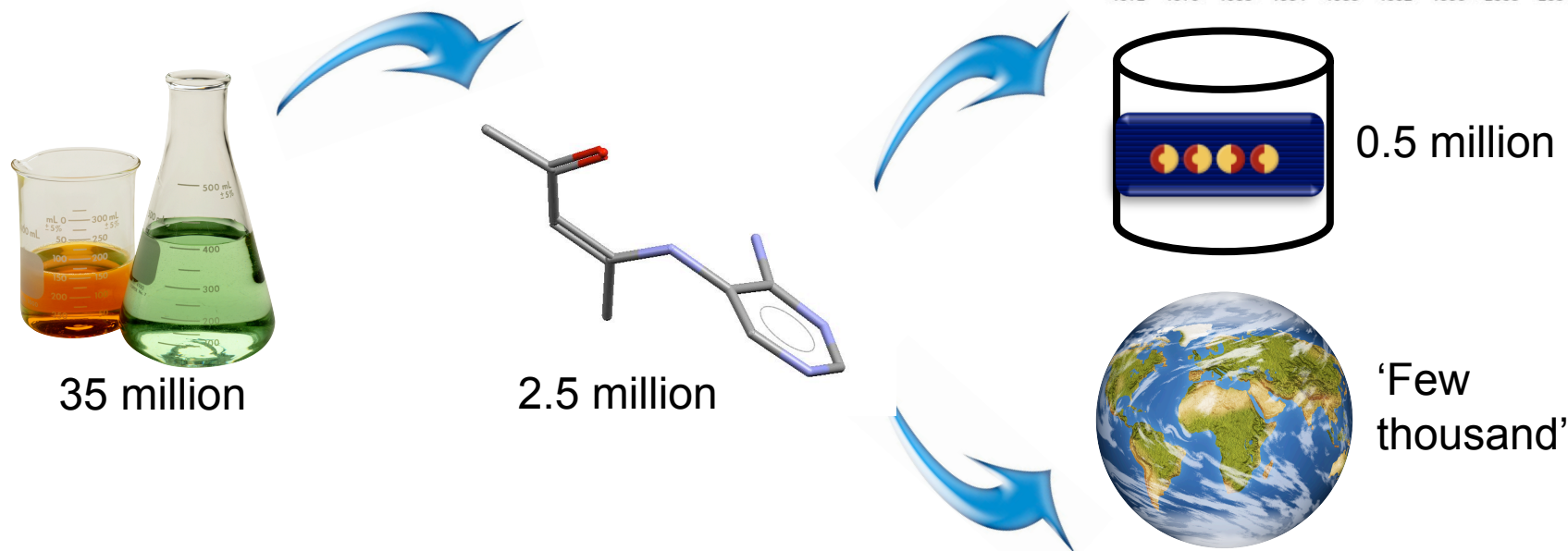
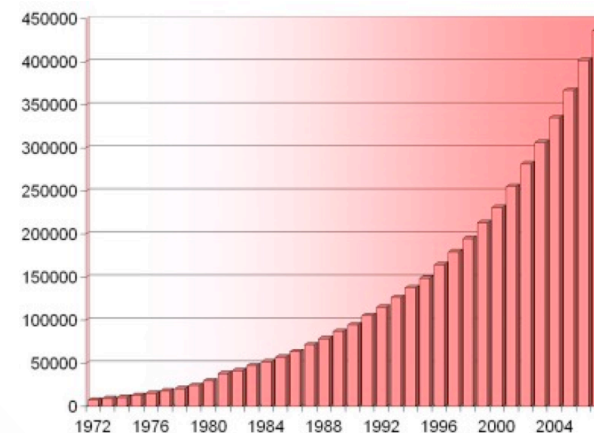
New Information Exchange Environments



- 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

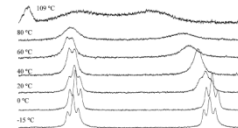


The primary cause is the current data publication process, which is tied to journal articles and peer review

Intellect & Interpretation
(Journal article, report, etc)

[illegible]

Fig. 5 Examples of compounds featuring C–F...H–N interactions, giving scalar H...F coupling constants



[Na₂O]₂·x[B(CN)₃BAr]₂][Ar⁺ = C₆F₅ (**4a**) or C₆F₄Me (**5a**)]. Although diacyanide anions have low lone pairs and is therefore theoretically capable of binding to three or possibly four borane molecules, only the diborates were obtained, even in the presence of excess BArAr₂ (Scheme 5). Colourless crystals of the sodium salts **4a** and **5a** were grown from diethyl ether but proved unsuitable for X-ray diffraction studies. Further reaction of the sodium salts with Ph₃CCl in dichloromethane afforded the trityl derivatives, [Ph₃C[B(CN)₃BAr]₂][Ar⁺ = C₆F₅ (**4b**) and C₆F₄Me (**5b**)]. The structure of **4b** is shown in Fig. 7. The *trans*-isomer of **5b** eventually yielded colourless crystals suitable for X-ray analysis which, however, once again turned out to be [C₆F₄Me]⁺[Ph₃P]⁻.

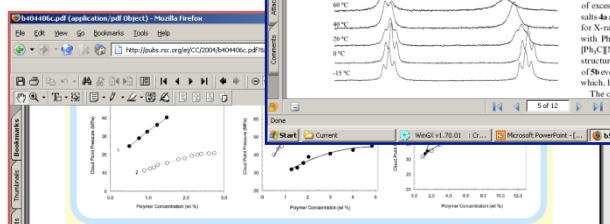
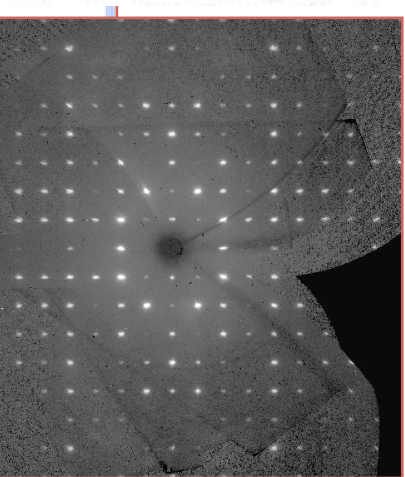
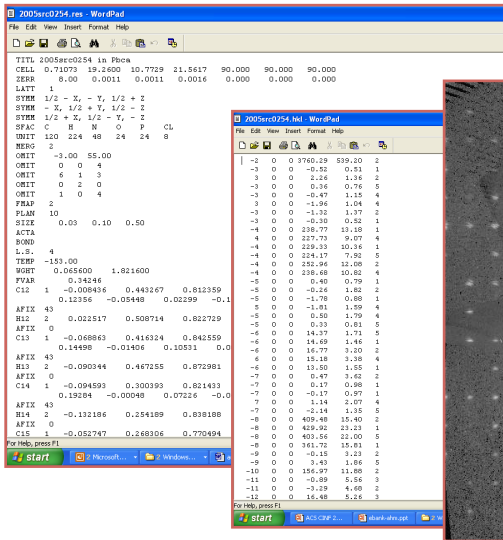
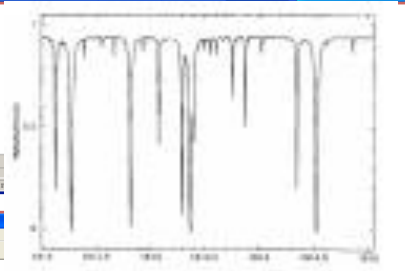
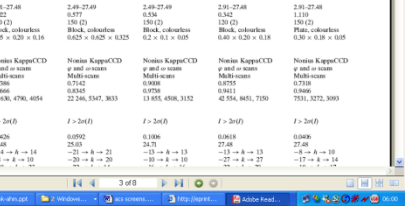
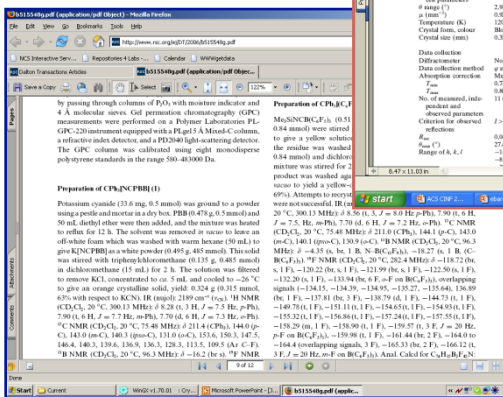
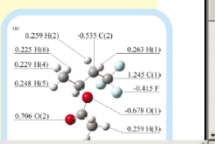


Fig. 2. (a) Phase behavior of (1) atactic polypropylene ($M_w = 425$), (2) polypropylene glycol monomethylether ($M_w = 1000$), in carbon dioxide at 295 K. (b) Phase behavior of oxygen-containing polymers in carbon dioxide at 295 K. (1) polypropylene glycol dimethyl ether, $M_w = 3500$, (2) polyvinyl methyl ether, $M_w = 3850$, (3) polyvinyl ethyl ether, $M_w = 3800$. (c) Phase behavior of oxygen-containing polymers in carbon dioxide at 295 K. (1) polyvinyl acetate, $M_w = 7700$, (2) polyvinyl ethyl ether, $M_w = 3800$, (3) polyvinyl acetate, $M_w = 3090$.

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 a decade²¹ that polymethyl acrylate (PMA) and polyvinyl acetate (PVAc) exhibit miscibility pressures in CO₂ that differ by hundreds of bar—this result would not be predicted by any group contribution thermodynamic model currently in use without purely empirical adjustments. Indeed, the PMA/PVAc effect is preserved even when

We believe that at least part of the answer to these puzzles lies in CO₂'s ability to act on both Lewis acid and Lewis base, coupled with subtle effects of neighboring substituents on the acidity of certain protons. For example, Wallen and colleagues²⁷ in an analysis of interactions between acetate groups and CO₂ found that the acidity of the methyl acetate



The eCrystals Data Repository

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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^c, Simon J. Coles^c and Susanne L. Huth^c

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

^aGebze Institute of Technology^a
^bBirkbeck College^b
^cUniversity of Southampton^c

C3H6Cl4N3O2P3

InChI=1/C3H12Cl4N3O2P3/c4-13(5)8-14(6,7)10-15(9-13)11-2-1-3-12-15/h6-10,13-15H,1-3H2

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

Controlled Keywords: cyclophosphazene, phase transition, variable temperature

Date Created: 28 March 2007

Deposited On: 21 Apr 2008 15:56

Deposited By: Dr Simon J Coles

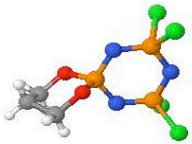
Data collection parameters

Chemical formula	C3 H6 Cl4 N3 O2 P3
Crystallisation Solvent	
Crystal morphology	Rod
Crystal system	Orthorhombic
Space group symbol	Pna2(1)
Cell length a	13.4604(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)
Export as: [EndNote](#) [BibTeX](#) [ASCII Citation](#)



Available Files

Final Result

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2005sjc0007.fcf	138k

Validation

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Solution

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Processing


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Data Collection


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Other Files

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2005sjc0007.ins	4k
2005sjc0007.mol	2k
2005sjc0007.p4p	1k
2005sjc0007_ellipsoid.gif	21k







 | **D | C | C** | 

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)
Export as: [EndNote](#) [BibTeX](#) [ASCII Citation](#)

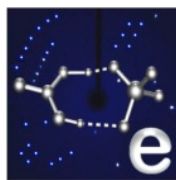
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- Quick & simple to deposit
- Software tools
- Laboratory archive
- Community involvement
- 'Embargo' facility
- Structured foundations
- Discoverable & harvestable

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

A Thorough Approach to Dissemination

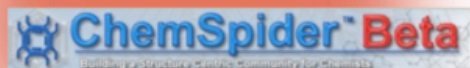
- Using simple Dublin Core protocol (OAI-PMH)
 - Crystal structure
 - Title (Systematic IUPAC Name)
 - Authors
 - Affiliation
 - Creation Date
- Additional **chemical** information through Qualified Dublin Core
 - Empirical formula
 - International Chemical Identifier (InChI)
 - Compound Class & Keywords
- 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>



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ChemSeer



CrystalEye (beta)

eBank UK



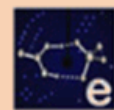
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RSC



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Nottingham



University
of Glasgow

Reciprocal Net



Science & Technology
Facilities Council

Useful Chemistry

JISC



EPSRC

Engineering and Physical Sciences
Research Council

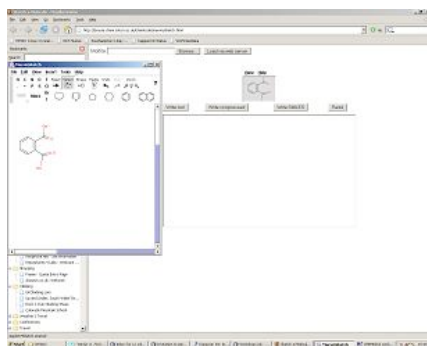


DCC

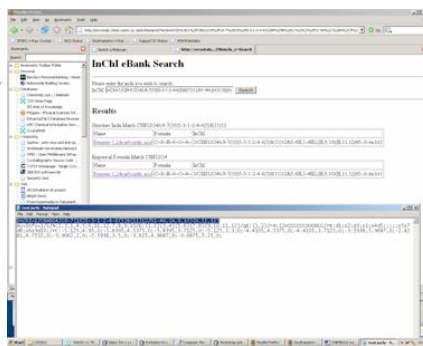
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Simple Integration into Teaching

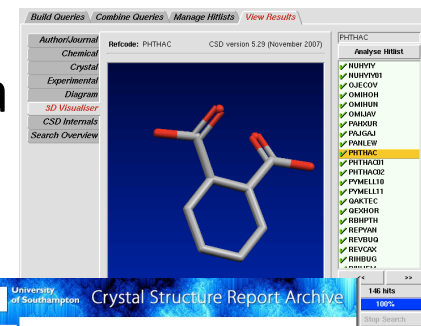
- Component of MChem course...using REAL data



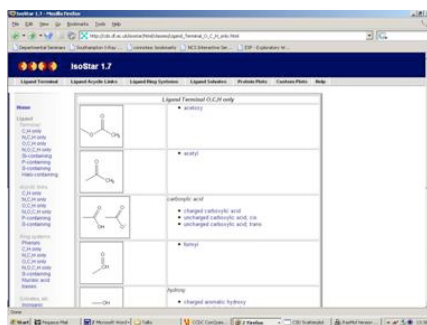
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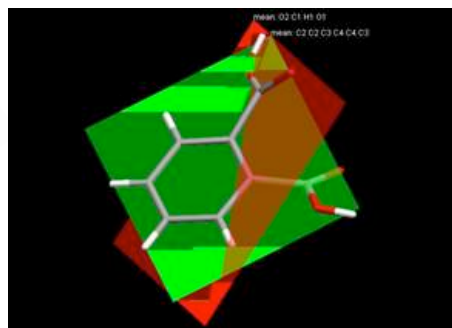
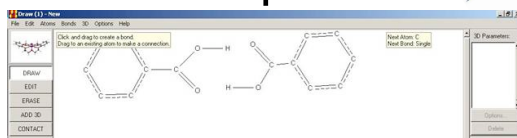
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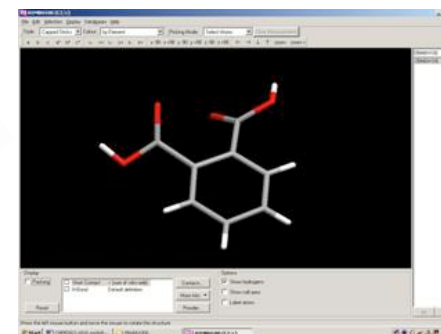
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Compare



Analyse



Manipulate

Open Science Experiment

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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

$C_9H_{11}N_1O_1$

InChI=1/C9H11NO/c1-7-3-5-9(6-4-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)

Identification Number: 10.3737/ecrystals.chem.soton.ac.uk/544

Controlled Keywords: para-substituted acetanilide

Date Created: 21 June 2008

Deposited On: 01 Aug 2008 17:29

Deposited By: Ms L.S. Huth

Data collection parameters

Chemical formula C9 H11 N O

Available Files

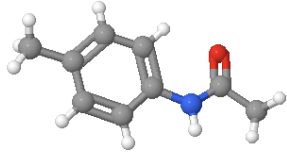
Final Result

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2008lsh008.cml	3k
2008lsh008.fcf	89k

Validation

2008lsh008_checkcif.htm	7k
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Jmol



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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

$C_{10}H_{13}N_1O_2$

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 Number: 10.3737/ecrystals.chem.soton.ac.uk/547

Controlled Keywords: para-substituted acetanilide

Date Created: 07 July 2008

Deposited On: 01 Aug 2008 17:45

Deposited By: Ms L.S. Huth

Data collection parameters

Chemical formula C10 H13 N O2

Available Files

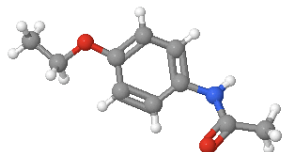
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Jmol



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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

$C_9H_{11}N_1O_2$

InChI=1/C9H11NO2/c1-7(11)10-8-3-5-9(12-2)6-4-8/h3-6H,1-2H3,(H,10,11)

Identification Number: 10.3737/ecrystals.chem.soton.ac.uk/543

Controlled Keywords: para-substituted acetanilide

Date Created: 21 June 2008

Deposited On: 01 Aug 2008 17:24

Deposited By: Ms L.S. Huth

Data collection parameters

Chemical formula C9 H11 N O2

Available Files

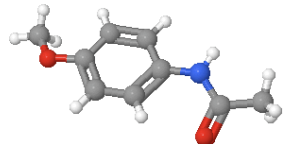
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Jmol



<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

Repositories 4 Labs - Welcome to Repositories 4 Labs
http://jet.ecs.soton.ac.uk/ Login

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

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

The disease has developed resistance to existing drugs

SEE ALSO:

- Fungus 'may help malaria fight' 09 Jun 05 | Health
- Malaria drug resistance warning 06 Jun 05 | Health
- Science shows how malaria 'hides' 08 Apr 05 | Health
- Global toll of malaria 'doubled' 10 Mar 05 | Health

RELATED BBC LINKS:

- Malaria - Global Menace

BBC Hampshire Information and features on the BBC Hampshire website

BBC Berkshire Information and features on the BBC Berkshire website

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

Current user: Simon Coles Log Out

The Drug Design Process

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 1

The first thing is to determine on existing treat conditions for which there treatments are designed cold and flu treatment, h

Step 2

The next question is how receptor pathway? Block hypothesis for treatment

Step 3

Next you need a compound chemists, pharmacologist organisms), and biologist may have other unwanted compounds are the natural disease. Some are discovered

@malaria
Home
CCDC
Lifecycle
e-Malaria Project
Background
Southampton
Schools
eScience
Publications
Malaria
Introduction
Symptoms
Treatments
Prevention
Target
Chemistry
Bonding
Hydrophilicity
Structure
Proteins
DHFR
Drug Discovery
eMalaria Tools
Projects
Molecules

Current user: Simon Coles Log Out

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:

1. Permanent dipole - permanent dipole
2. Permanent dipole - induced dipole
3. 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 a 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.

Current user: en two atoms

Hydrophilicity Test

Check your understanding of hydrophilicity below.

@malaria

		Mark
H-H		<input type="radio"/>
Cl-H		<input type="radio"/>
		<input type="radio"/>

Task: You must sort Polar and Non-Polar

Polar	Non-Polar

Chemistry
Bonding
Hydrophilicity
Structure
Proteins
DHFR

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

Open Science Experiment

@malaria

Insert Molecule

Molecule Name: N-(4-methylphenyl)acetamide

File Edit View Insert Tools Help

H C N O P S Cl Br I More

Chemical structure of N-(4-methylphenyl)acetamide is shown.

3Crystals

Home About Browse by Year Browse by People

Login Create Account

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. Cole^a

University of Southampton^a

C₉H₉N₁O₁

InChI=1/C9H11NO/c1-7-3-5-9(6-4-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)

Identification Number: 10.3737/crystals.chem.soton.ac.uk/544

Controlled Keywords: para-substituted acetamide

Date: 21 June 2008

Created: 01 Aug 2008 17:29

Deposited On: 01 Aug 2008 17:29

Deposited By: Ms L.S. Huth

Data collection parameters

Chemical formula: C9 H11 N O

Available Files

File	Size
2008sh008.cif	11k
2008sh008.cml	3k
2008sh008.fcf	89k
2008sh008_checkoff.htm	7k

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@malaria

Molecule N 4 methylphenyl acetamide

Chemical structure of N-(4-methylphenyl)acetamide is shown.

Id 9213

Name N 4 methylphenyl acetamide

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

InChI InChI=InChI=1/C9H11NO/c1-7-3-5-9(6-4-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)

Status 3D

Jobs 0/0 (0.00:0.00)

Add a Docking Job to target (Malaria DHFR) [add]

Jobs

Id	Status	Run Time	H-Bonds	Wdv	Strain	Energy	Tools
23572	Done	11s	5.53	-4.89	37.59		

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



@malaria

Molecules - SColes

Sort By Entered Order

Insert Molecule

Id	Name	Smile	Image	Status	Jobs	Tools
9215	N 4 ethoxyphenyl acetamide	CCOC1=CC=C(C(=O)N)C=C1		3D	1/1 (41.74:41.74)	
9214	N 4 methoxyphenyl acetamide	COC1=CC=C(C(=O)N)C=C1		3D	1/1 (37.01:37.01)	
9213	N 4 methylphenyl acetamide	CC(=O)NC1=CC=C(C)C=C1		3D	1/1 (37.59:37.59)	
8997	ala-asn-gln	[NH3+][C@@H](C(=O)N)C(=O)N		3D	1/1 (49.92:49.92)	

Insert Molecule **Insert Peptide**

© University of Southampton 2005

@malaria

Molecule N 4 methylphenyl acetamide

Chemical structure of N-(4-methylphenyl)acetamide is shown.

Id 9213

Name N 4 methylphenyl acetamide

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

InChI InChI=InChI=1/C9H11NO/c1-7-3-5-9(6-4-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)

Status 3D

Jobs 1/1 (37.59:37.59)

Add a Docking Job to target (Malaria DHFR) [add]

Jobs

Id	Status	Run Time	H-Bonds	Wdv	Strain	Energy	Tools
23572	Done	11s	5.53	-4.89	37.59		

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

3D View

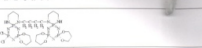
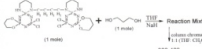
dark blue green off pale blue black whiteBackground

CPK GreenTop CyanRight

Drug Molecule

CPK GreenTop CyanRight

General Chemistry Issues: Data Generation

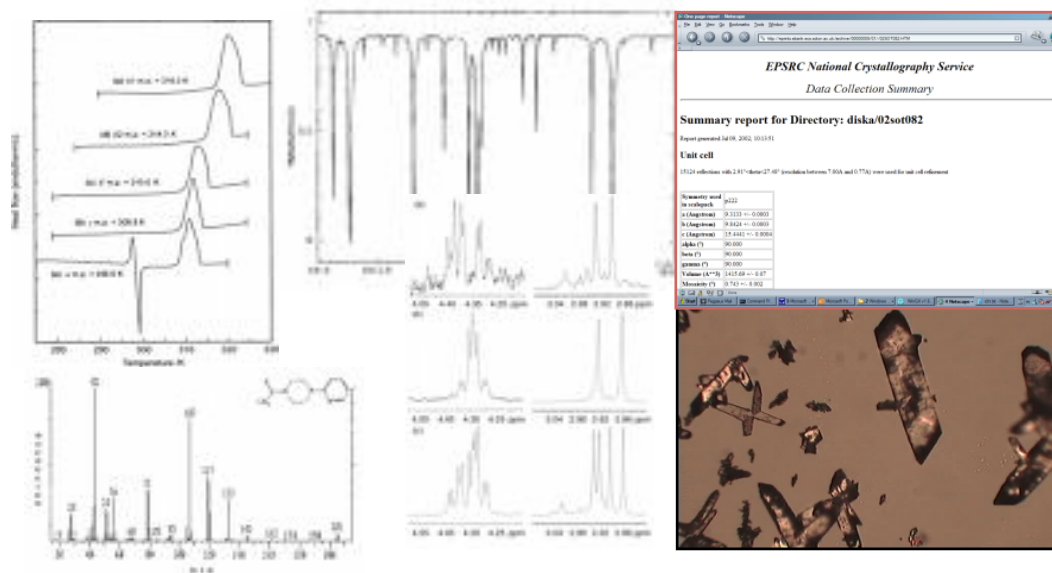
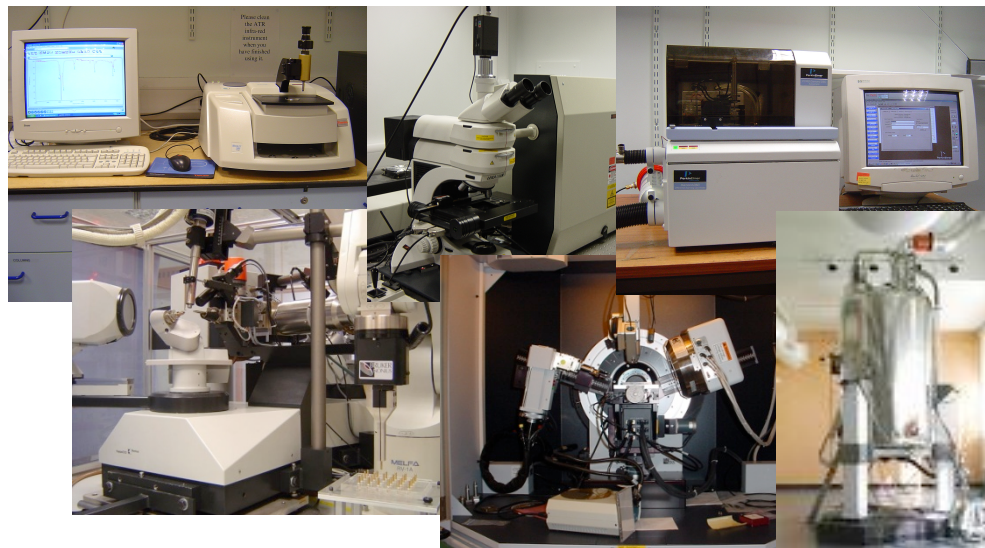
Compound Details		For X-ray	22.05.2004
Researcher:	Goni VENEZUELA CRTU		
Code:	303-489-a		
Compound:	<chem>C12H16N2O4</chem>		
Empirical Formula:	<chem>C12H16N2O4</chem>		
Proposed Formula:	<chem>C12H16N2O4</chem>		
Structural Formula:			
Melting Point (°C):	303-489-a (mp 132-133 °C)		
Reagent (and its purity if relevant):	1,3-propanediol, triethylamine, NaH, dichloromethane, Hexane, EtOAc		
General Properties (e.g. high thermal stability, solvent, moisture sensitivity):	This product is soluble in CH ₂ Cl ₂ , CH ₂ Cl ₂		
Crystallization Solvent:	CHCl ₃ /Hexane EtOAc (1:1:2)		
Appearance of Recrystallized Compound:	White solid		
Yield:	Cal: 303-489-a (76%)		
Elemental Analysis:	C, H, N		
Calculated:	C: 58.5, H: 6.5, N: 3.5		
Found:	C: 58.5, H: 6.5, N: 3.5		
Reaction Scheme:			
Notes:	303-489-a (mp 132-133 °C)		
Yield:	76%		



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”

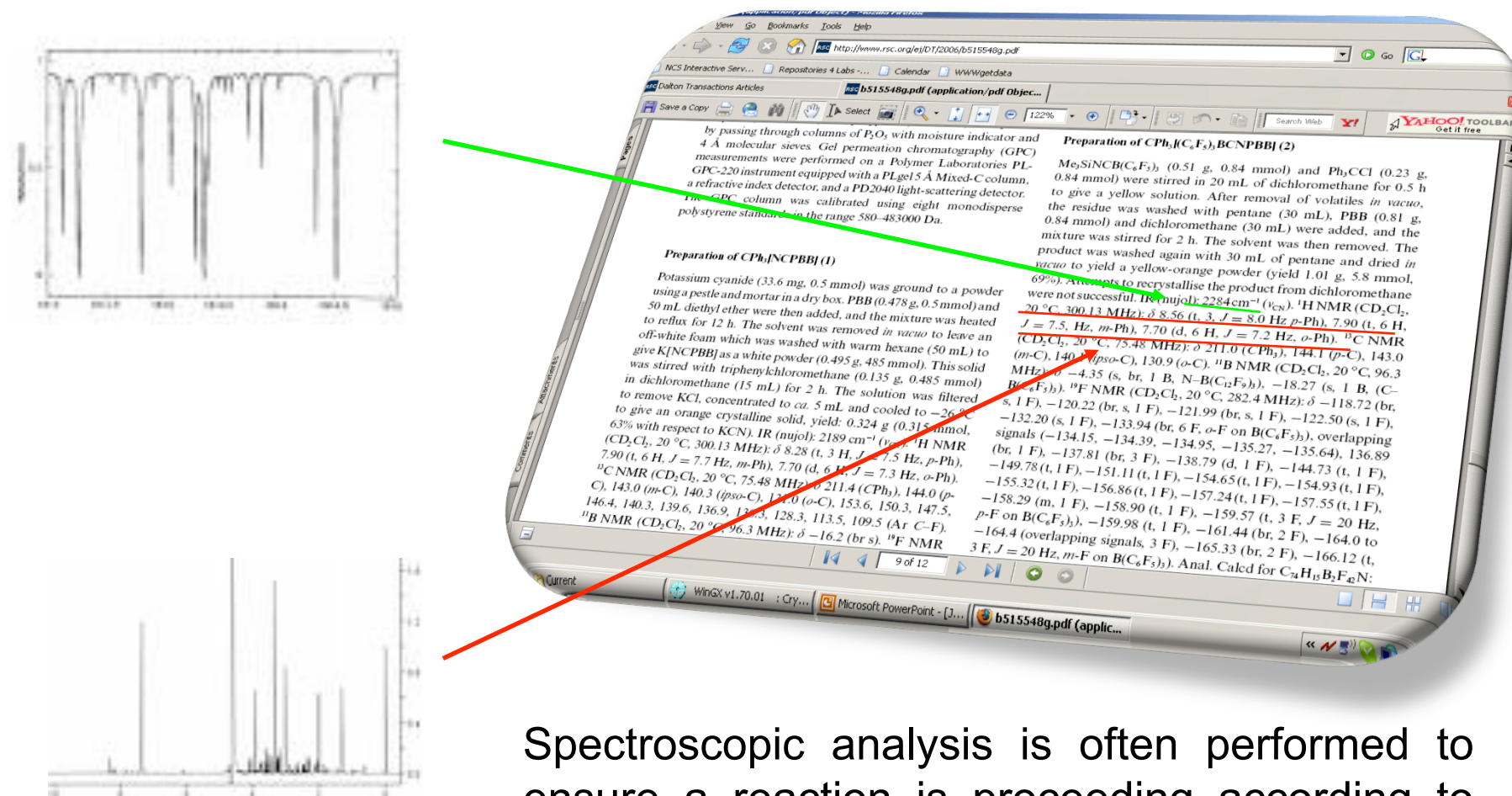
“Lost in some research assistant’s computer, the data are often irretrievable or an undecipherable string of digits”

“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)

The screenshot shows a web form for creating a new compound record. It includes fields for 'Name' (with examples like 2-acetylglutamic acid and aspirin), 'Identifier' (with example TLT/1142), and a 'Sketch' section with a Marvin Sketch app icon. Below these are 'Collaborators' fields for Family Name, Given Name, Initials, and Email address, with two entries: Coles, Simon J. and Hursthouse, Michael B. There is also a 'More Spaces' button. On the right, a chemical structure is displayed, showing a benzene ring with a chlorine atom, an amine group, and a thioether group.

Add new experiment type

The screenshot shows a web form for adding a new experiment type. It has two main sections: 'Add New Compound' and 'Add Experiment'. The 'Add New Compound' section includes fields for 'Enter metadata describing a new compound' and 'Experimental results'. The 'Add Experiment' section includes a dropdown menu for 'Experiment Type' with options like Single Crystal Diffraction, Powder X-Ray Diffraction, IR, UV-Vis, Mass Spec, Raman, Optical Microscopy, DSC, TGA, NMR, Solid State NMR, SHG Laser Spectroscopy, Elemental Analysis, and Add Experiment. There are also 'show details' links for each option. At the bottom, there are 'User Options' and a 'change your user record' link.

Add metadata and
upload data files

The screenshot shows a web form for adding metadata and uploading data files. It includes a list of 'Reference Material' with examples like Indium, Lead, and Aluminum. Below this are fields for 'Pan Bottom', 'Pan Lid', and 'Purge Gas', each with a dropdown menu and examples. There are also 'More Spaces' buttons.

The screenshot shows a web form for adding metadata and uploading data files. It includes a 'Compound' field with a dropdown menu and a 'Date' field with a dropdown menu. There are also 'Previous', 'Save for Later', and 'Next' buttons. At the bottom, there is a 'Location' field with a dropdown menu.

Open Science Experiment

R4L Repository for the Laboratory
 Home About Browse Search Register User Area Help

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 the instrument from the list below:

DSC: Mettler Toledo DSC 823e
 DSC: Mettler Toledo MultiSTAR 1935
 DSC: Mettler Toledo MultiSTAR 1937
 DSC: Parkin-Elmer Diamond DSC
 DSC: TA Instruments Q2000 DSC
 DSC: TA Instruments Q2000 DSC
 DSC: TA Instruments Q2000 DSC
 DSC: TA Instruments Q2000 DSC
 IR: BTEC200 NIR Fiber Coupled InGaAs Spectrometer
 IR: Beijing Scientific Instruments & Materials Corp. FT-IR

Reference Material

The reference material used:
 Example: Indium
 Example: Lead

Pan Bottom

The type of pan bottom used:
 Example: aluminum
 Example: graphite
 Example: platinum

Pan Lid

The type of pan lid used:
 Example: vented aluminum

Purge Gas

The type of purge gas used:
 Example: helium

Edit Item: Document File Upload

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 Stop Editing Format Finished >

Adding files for format: Other (JDX Spectrum)

These are the files you have uploaded for this format:

TLT544/2 144 Kb [Delete] [Make Primary]
 TLT544/2 28 Kb [Delete] This is the primary file. The link from the summary page will point to this file.
 [Delete All Files]

Upload a file from your PC

Type of file being uploaded: Normal File [v] Browse...

Select a file to upload:

Upload File

Capture a file from a URL

Enter a URL to capture a file from: http://

Capture File

< Previous Stop Editing Format Finished >

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_gherh	show details sign off
ganw_htrs	show details sign off
TLT71142 Paracetamol	show details sign off
TLT538/2 N-(4-methylphenyl)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

Add Experiment... Add sign off

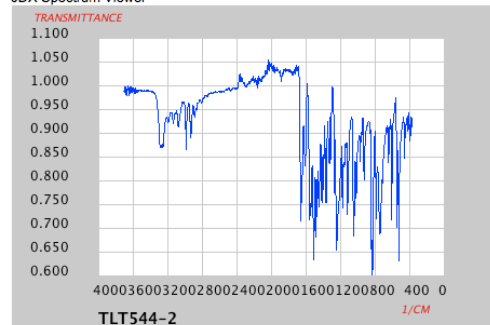
*IR (08 August 2008 14:10)
 *DSC (11 August 2008 16:00)
 Optical Microscopy (08 August 2008 15:30)

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 \[9 Kb\]](#)

JDX Spectrum Viewer



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

Location: 30:3067

ID Code: 396

Deposited By: [Dr Simon Coles](#)

Deposited On: 08 August 2008

Repository Staff Only: [edit this](#)

Contact Information

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: 396

Deposited By: [Dr Simon Coles](#)

Deposited On: 08 August 2008

Experimental Results:

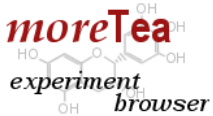
- [*IR \(08 August 2008 14:10\)](#)
- [*DSC \(11 August 2008 16:00\)](#)
- [Optical Microscopy \(08 August 2008 15:30\)](#)

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

Contact Information

<http://r4l.eprints.org>

A New Kind of Electronic Lab Notebook



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.

Edit Material

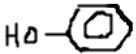
Description
Solid phenol

Ratio Atomic Weight

Safety Notes
Toxic by ingestion and skin absorption phenol from the bottle because the sol gloves and work in a fume cupboard.

9.4 g Solid phenol

Observations/Notes



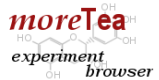
Terms of Use

© University of Southampton IT Innovation Centre 2007

Add Experiment


Name Identifier

Description



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)**

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 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

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

ajb512555 [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
Not Known, Treat as toxic

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 60 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. (0.75 g/mL, 101.2 g/mol)

Procedure

1.

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.



moreTea Lab Tool [CN=Andrew Bailey, OU=Che...]

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

Summary Measure

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

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

moreTea Lab Tool [CN=Andrew Bailey, OU=Che...]

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

Summary Measure

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

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

Atomic Weight	Amount
255.1	Required 1.1 g
COSHH Information	Used 1.1483 g
Not Known, Treat as toxic	

moreTea Lab Tool [CN=Andrew Bailey, OU=Che...]

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

Summary Measure

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

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

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

moreTea Lab Tool [CN=Andrew Bailey, OU=Che...]

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

Summary Measure

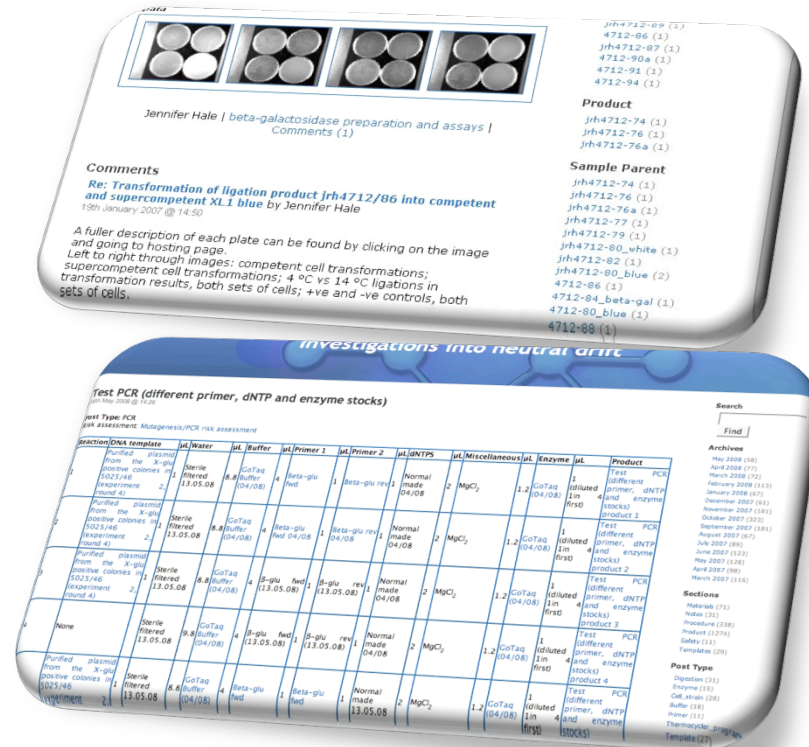
Procedure - Step 7 of 10
The Organic layer was retained and was washed with further water (2 x 50 mL)

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

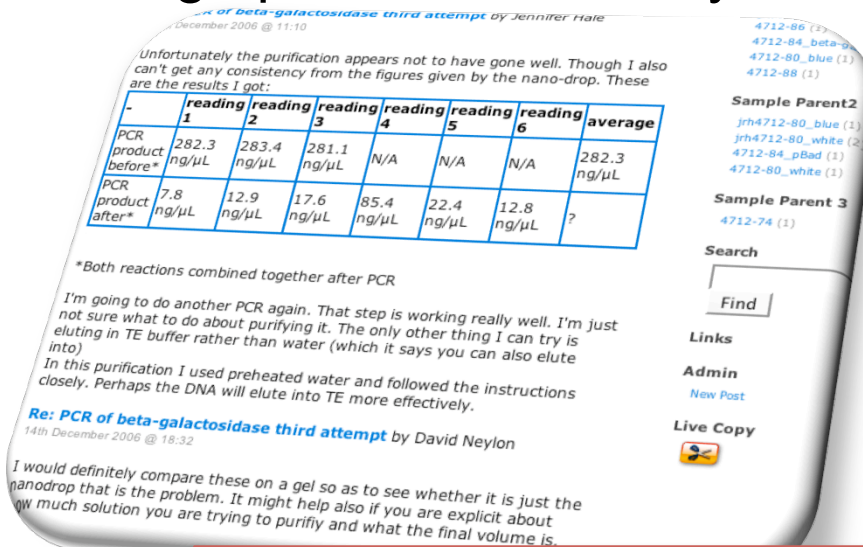
Analysis & Discussion: Blogging Experiments

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

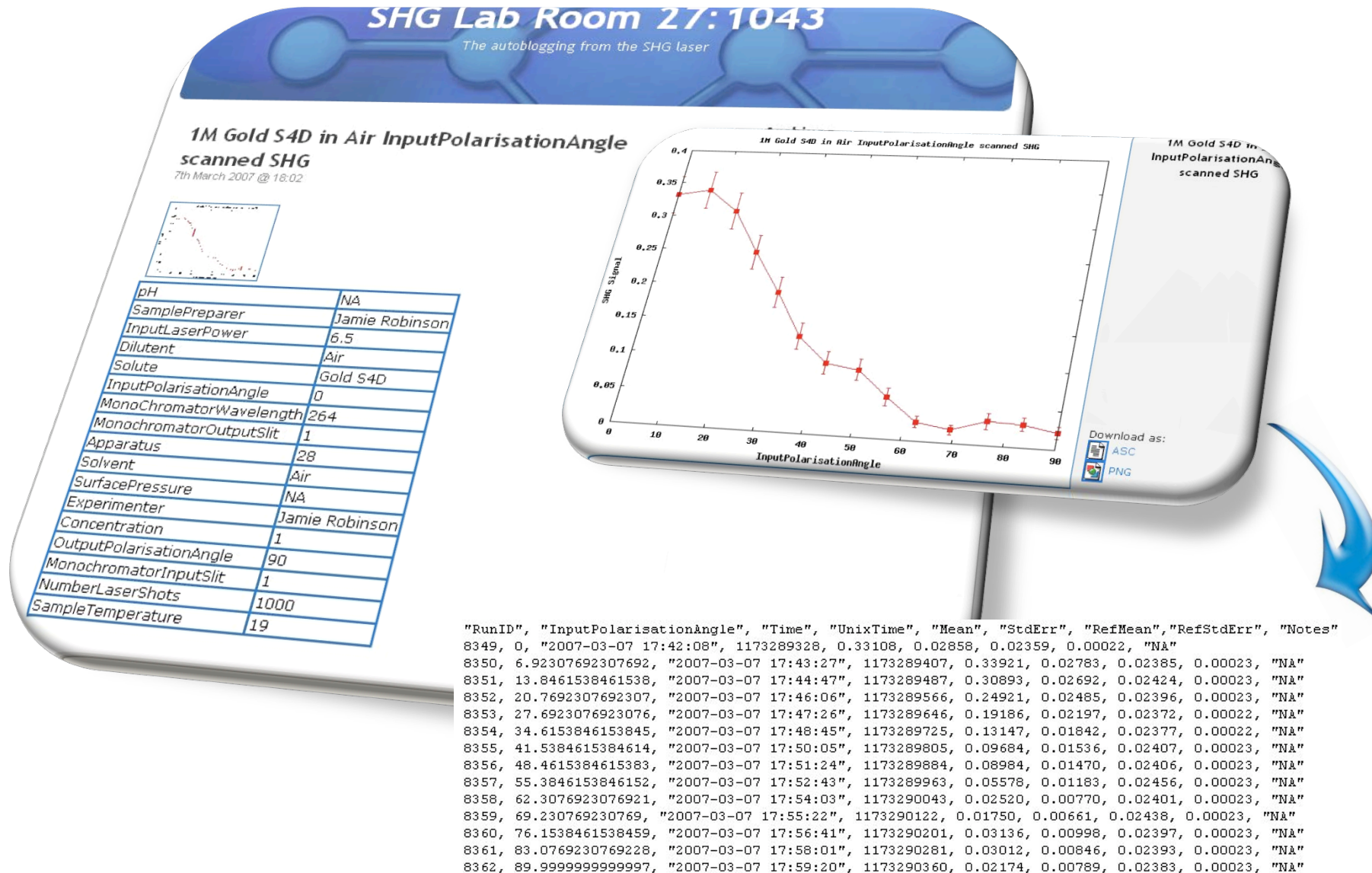


- Enables 'geographically distributed collaborative research'
- Can be open or private
- A useful approach for sharing 'failed' experiments?



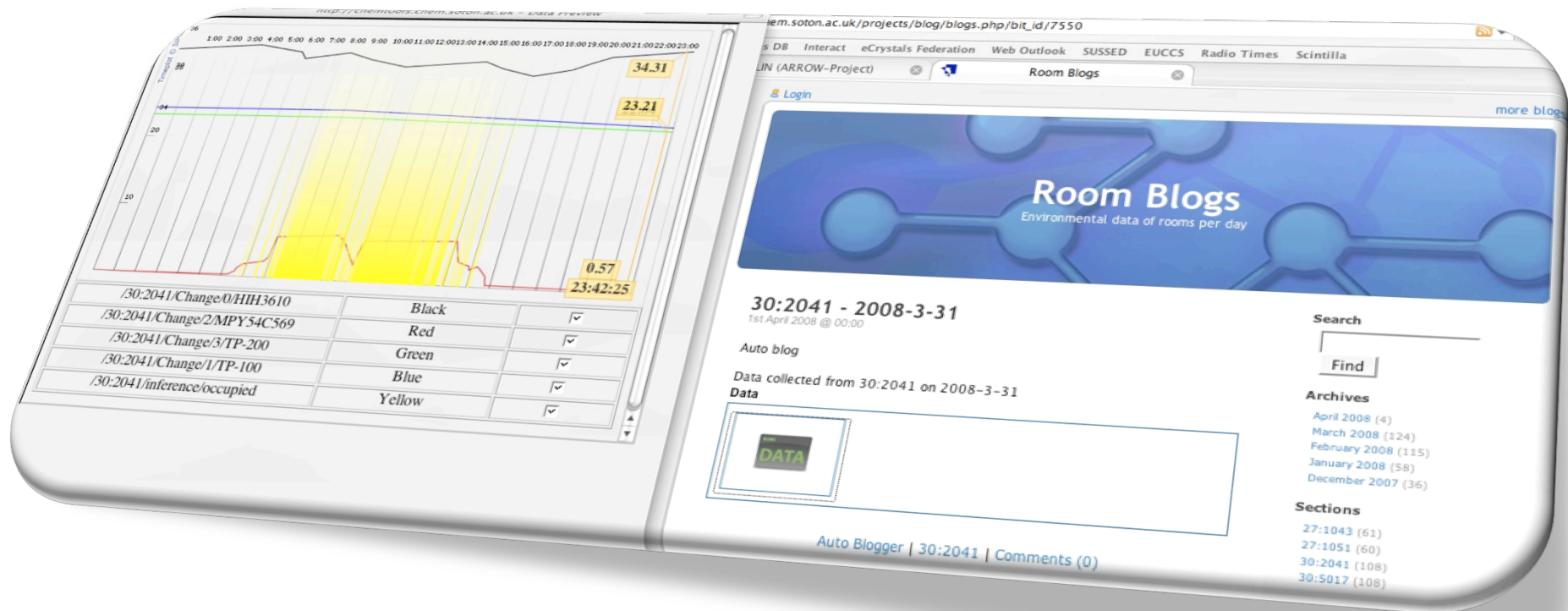
<http://chemtools.chem.soton.ac.uk/projects/blog/>

Automatic Blogging by Machines



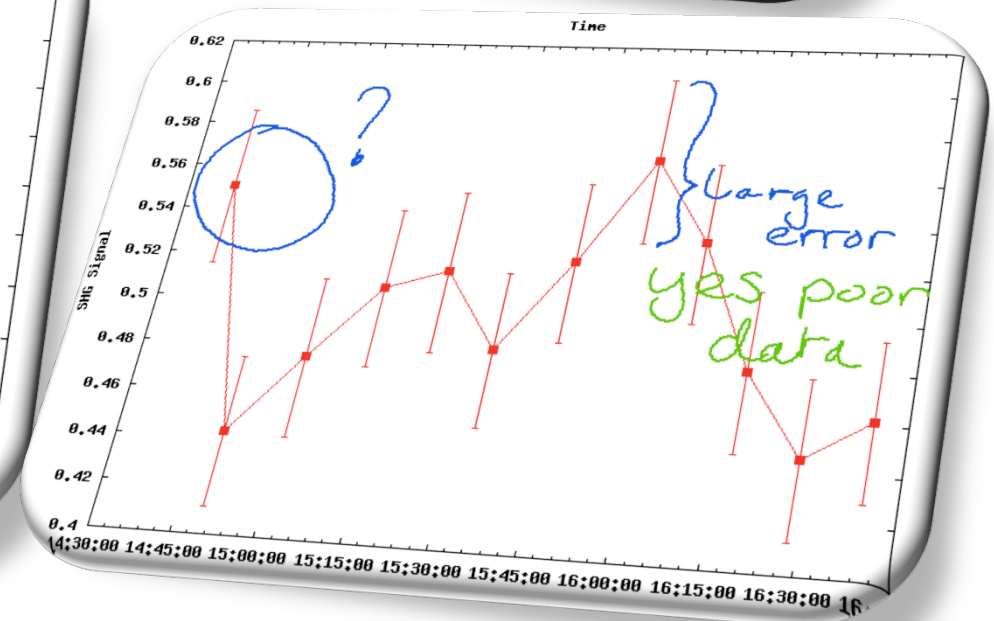
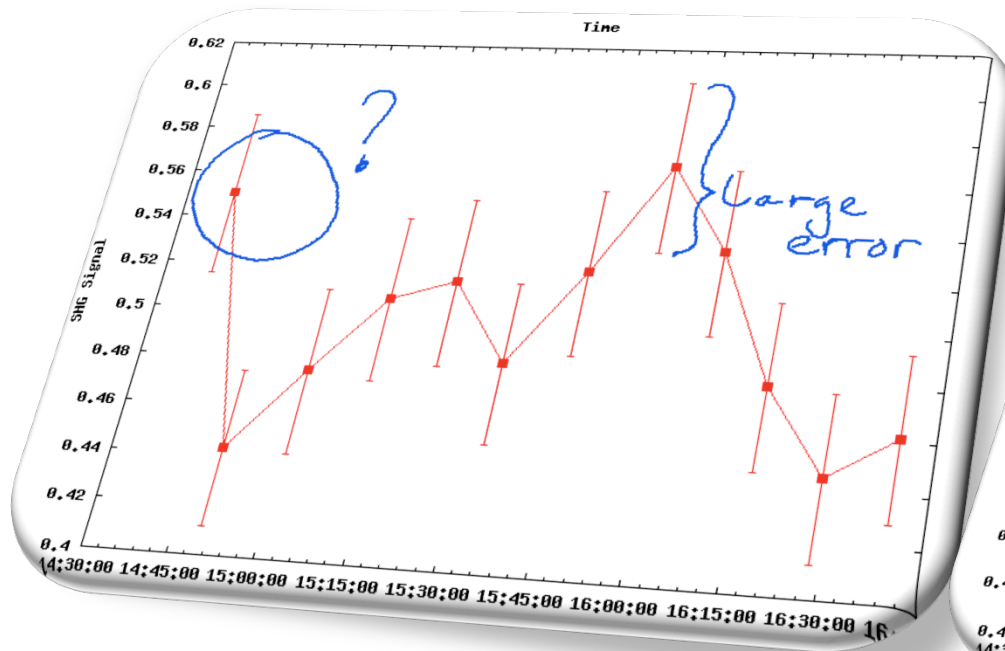
Automatic Blogging by Sensors

- 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

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

Group: Structural Systematics and Structure-Property

Key: Creators value: Simon_Coles

Key: Experiment Type value: Hot_Stage_Microscopy

Reason For Edit: Submit Preview

or upload data

Search

Admin
New Post

Archives
August 2008 (3)
July 2008 (3)

Sections
Development (3)
Structural Systematics and Structure-Property (3)

Creators
Simon_Coles, Ryan_Warnock (1)
Terry_Threlfall (1)
Simon_Coles (3)

Experiment Type
Synthesis (1)
Infra-Red (1)
Crystal_Structure (1)
Hot_Stage_Microscopy (2)
DSC (1)

Misc
Show/Hide Keys

Live Copy

N-(4-methoxyphenyl)acetamide HSM
15th August 2008 @ 13:08

Creators: Simon_Coles
Experiment Type: Hot_Stage_Microscopy
Deposited at: <http://r4i-dev.eprints.org/395/>
Acetylation of amines - general synthetic route



Simon Coles | Edit Post | Structural Systematics and Structure-Property | Comments (0)

N-(4-methoxyphenyl)acetamide DSC
15th 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
methoxyphenyl)acetamide Crystal Structure
N-(4-ethoxyphenyl)acetamide structure

Simon Coles | Edit Post | Structural Systematics and Structure-Property | Comments (0)

ecrystals

Acetylation of amines - general synthetic route
18th 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 aniline with glacial acetic acid, preferably in the presence of a trace of mineral acid and distilling off (azeotroping) the water. However this will only work if the amine has a convenient boiling point and is 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 more powerful still. 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 and some were weakly basic. Acetyl chloride was chosen as the acetylation agent. Pyridine was used as the solvent because it is a powerful solvent which catalyses the acetylation process. However, acetyl chloride and pyridine react vigorously together. So the following procedure was adopted: a 1:1 molar mixture of acetic anhydride and acetyl chloride was prepared. In each case the amine (10 millimoles i.e. about a gram) was dissolved in about 4 ml of pyridine and 1ml of the acetylation mixture (approximately 1.2 mol equivalents) was added slowly from a pipette. The reaction mixture was heated to boiling and evaporated in a stream of nitrogen until copious fumes appeared. These are pyridinium chloride, which is extraordinarily volatile. This is another advantage of using pyridine with acetyl chloride as it and the hydrogen chloride produced in the reaction are readily removed. The residue was allowed to cool, and water, ca. 10ml was added. 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 anilides are rather too soluble and above procedure is vigorous and so is suitable only for the small scale used here.

This Post is Linked By: N-(4-methylphenyl)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 DSC; N-(4-methoxyphenyl)acetamide HSM; N-(4-methylphenyl)acetamide Hot Stage Microscopy; N-(4-ethoxyphenyl)acetamide Hot Stage Microscopy; N-(4-methoxyphenyl)acetamide Infra-Red.

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Structural Systematics and Structure-Property (13)

Creators
Simon_Coles, Ryan_Warnock (1)
Terry_Threlfall (1)
Simon_Coles (12)

Experiment Type
Synthesis (1)
Infra-Red (3)
Crystal_Structure (3)
DSC (2)
eMalaria_docking_job (1)
Hot_Stage_Microscopy (3)

Misc
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Open Science Experiment

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](#) DSC [N-\(4-ethoxyphenyl\)acetamide](#) DSC [N-\(4-methylphenyl\)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-\(4-ethoxyphenyl\)acetamide](#) Hot Stage Microscopy[N-\(4-methoxyphenyl\)acetamide](#) HSMN-[N-\(4-methylphenyl\)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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Creators

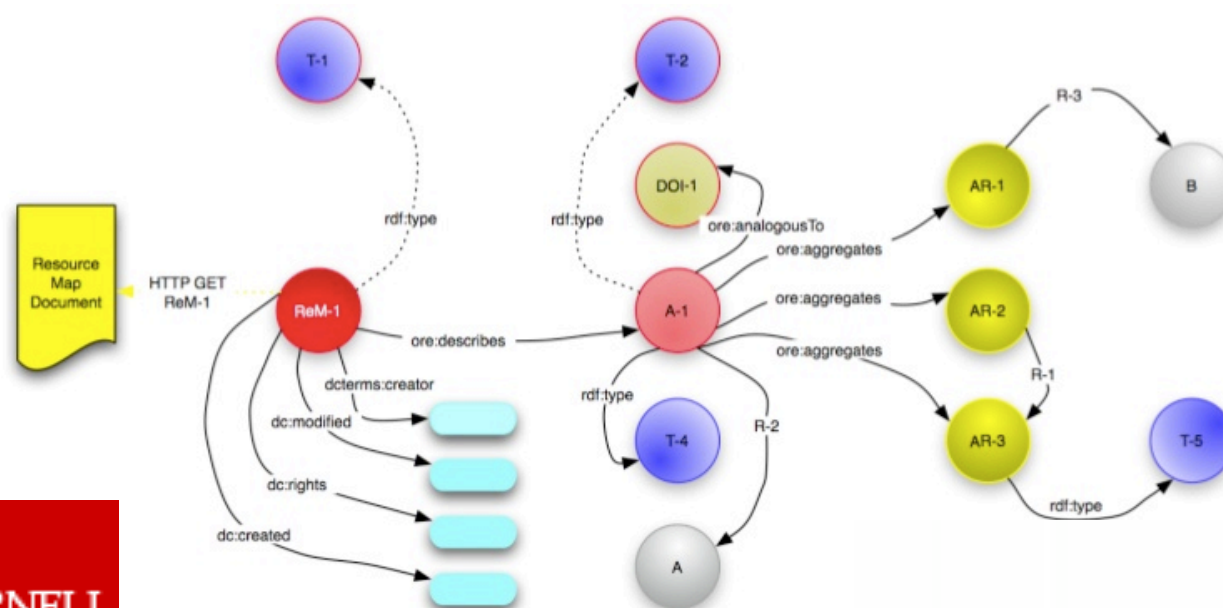
[Simon_Coles](#), [Ryan_Warnock \(1\)](#)
[Terry_Threlfall \(1\)](#)
[Simon_Coles \(14\)](#)

Experiment Type

[Synthesis \(1\)](#)
[Infra-Red \(3\)](#)
[Crystal_Structure \(3\)](#)
[DSC \(3\)](#)
[eMalaria_docking_job \(1\)](#)
[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



'Sharing Experiments'

The screenshot displays the myExperiment website interface. At the top, the logo "my experiment beta" is visible, along with navigation links for Wiki, Mailing List, Publications, Logout, Give us Feedback, and Invite. Below the logo, a navigation bar includes Home, Users, Groups, Workflows, Files, and Packs. A search bar is located in the center of this bar. The main content area is divided into several sections:

- Home »**: A yellow banner at the top of the main content area states "Logged in successfully. Welcome to myExperiment!".
- myExperiment currently has 1079 users, 91 groups, 329 workflows, 113 files and 20 packs**: A yellow banner below the login message.
- Site Announcements**: A section on the left containing several announcements, including "myExperiment design paper published", "Significant changes to Biomart filters and attributes! Please check your workflows!", "myExperiment has 1000 registered users", "New myExperiment and WHIP plugin for Taverna", and "wiki.myexperiment.org new and improved for developers".
- My News**: A section in the center stating "No news".
- Updated Items**: A section in the center listing recent updates, including files, packs, and workflows, such as "Article List Viewer Blocks by Jiro", "Genbank Cross Reference Blocks by Jiro", "Provenance challenge by Paul Fisher", "A Test of myExperiment's file uploading by Yiming Sun", "An Introduction to Taverna and myExperiment - Background by Paul Fisher", "A Taverna Users Guide by Paul Fisher", "Newcastle NeuroScience by Paul Fisher", "Perfrom a text based search through PubMed by Paul Fisher", "random workers ages data by Ptimus", and "Random workers ages generated by Ptimus".
- New/Upload**: A section on the right with a "Workflow" dropdown and a "GO" button.
- Simon Coles**: A user profile section on the right showing a profile picture and a list of links: My Profile [edit], My Messages, My Memberships, My History, and My News.
- My Stuff**: A section on the right showing "2 friends | 0 groups | 1 Blogs | 2 Files".
- Friends**: A section on the right listing "David De Roure" and "Sacha Brostoff".
- Blogs**: A section on the right listing "Chemistry Stuff".
- Files**: A section on the right with a list of files.
- My Favourites**: A section on the right showing "0 favourites".
- My Tags**: A section on the right with a list of tags.

A red box at the bottom of the page contains the URL <http://www.myexperiment.org/>.

Open Science Experiment

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Home » Packs » acetanilide comparison study (test)

BOOKMARK

Item successfully added to pack.

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Pack: acetanilide comparison study (test)

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

[Add an item | Sharing | Tags (5) | Featured in Packs (0) | Favourited 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 @ 18:00:50)

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

[Add a comment here]

Added by Simon Coles ... 2 minutes ago (18/08/08 @ 18:00:32)

IR, DSC, HSM

Added by Simon Coles ... 2 minutes ago (18/08/08 @ 18:00:32)

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

[Add a comment here]

Added by Simon Coles ... 6 minutes ago (18/08/08 @ 18:04:58)

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)

IR, DSC, HSM

Added by Simon Coles ... 9 minutes ago (18/08/08 @ 18:01:38)

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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Quick add: (a link)

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Add

Quick add: (from your stuff)

File: 04sjc0831.cml

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Advanced add:

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Pack

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Simon Coles

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disease | ebi | example | kegg

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protein | protein annotation

sequence similarity search | shim

taverna | text mining | text_mining

text_mining_network | VL-e

1 item in this pack

Tags (5)

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

[edit]

Add Tags

Tags from Items (0)

None

Tags from Items (0)

None

Shared with Groups (0)

None

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None

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Favourited By (0)

No one

Add to your Favourites

Statistics

17 viewings

5 tags

0 favourites

0 comments

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Sharing Permissions (who can view and download)



[Edit Profile Picture]

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

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Simon Coles has been credited 0 times

Simon Coles has an average rating of:
0.0 / 5
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for their items

Description/summary not set

Other contact details:

Not specified

Interests:

Not specified

Field/Industry: Chemistry Academic Research

Occupation/Role(s): Academic

Organisation(s):

University of Southampton

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Note: some items may not be visible to you, due to viewing permissions.

Creator:



Simon Coles

acetanilide comparison study (test)

View

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

Comments: 0 | Viewed: 18 times |

Tags:

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

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protein | protein annotation

sequence similarity search | shim

taverna | text mining | text_mining

text_mining_network | VL-e

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

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- Mike Hursthouse, Jeremy Frey, Cameron Neylon, Andrew Milsted, Richard Stephenson, Jamie Robinson, Steven Wilson, Andrew Bailey, Mark Borkum



- Dave DeRoure, Les Carr, monica schraefel, Chris Gutteridge, Tim Myles-Board, Arouna Woukei, Dave Tarrant, Stuart Middleton



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

