

Open Notebook Science

NASA

Goddard Space Flight Center

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Drexel University

April 15, 2009

Open and Closed Science

Traditional
Lab Notebook
(unpublished)

Traditional
Journal
Article

Open Access
Journal Article

Open Notebook
Science (full
transparency)

RESEARCH

CLOSED



OPEN

TEACHING

Traditional
Paper
Textbook
F2F lectures

Lectures
Notes
public

Assigned
problems
public

Archived
Lectures
Public and
free online
textbooks



WIKIPEDIA
The Free Encyclopedia

Open Notebook Science

From Wikipedia, the free encyclopedia

Open Notebook Science is the practice of making the entire primary record of a research project publicly available online as it is recorded. This involves placing the personal, or laboratory, notebook of the researcher online along with all raw and processed data, and any associated material, as this material is generated. The

References

- [^] ^a ^b Goetz, T. Freeing the Dark Data of Failed Scientific Experiments *Wired Magazine*, Sept.25, 2007. [↗](#)
- [^] Sanderson, K (September 2008). "Data on display". *Nature*. doi:10.1038/455273a [↗](#).
- [^] Singh, S. (April 2008). "Data on display". *Cell*. doi:10.1016/j.cell.2008.04.003 [↗](#).
- [^] Lloyd, R. Era of Scientific Secrecy Near End *Live Science*, Sept 2, 2008. [↗](#)
- [^] Williams, A. J. Internet-based tools for communication and collaboration in chemistry *Drug Discovery Today*, vol 13, p. 502 (2008). [↗](#)
- [^] Everts, S. Open Source Science, *Chemical & Engineering News*, July 2006, 84 (30) p. 34. [↗](#)

Motivation: **Faster Science**, Better Science

Open Notebook Science Logos (Andy Lang, Shirley Wu)

Sharing: how much and when



<http://onsclaims.wikispaces.com/>

Where is Science headed?



WE ARE HERE

There are NO FACTS,
only measurements embedded
within assumptions

Open Notebook Science maintains
the integrity of data provenance by
making assumptions explicit

TRUST



PROOF

The solubility of 4-chlorobenzaldehyde

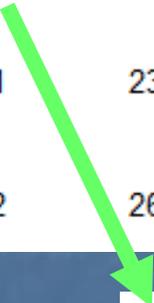


<http://usefulchem.wikispaces.com/Exp208>

ID	Solute	Solvent	Saturated Soln Conc (M)	BP(predicted from ChemSpider at 760mmHg)	BP (Predicted at 0.1T)
21b	3,4-dimethoxybenzaldehyde	Chloroform	5.44	281 °C	67.9 °C
25b	4-hydroxybenzaldehyde	Chloroform	1.75	246.6 °C	43.1 °C
27b	2-chloro-5-nitrobenzaldehyde	Chloroform	2.90	290.3 °C	74.6 °C
28b	4-chlorobenzaldehyde	Chloroform	0.07	213.7 °C	19.3 °C
29b	2,6-dichlorobenzaldehyde	Chloroform	3.41	239.2 °C	37.8 °C
30b	p-dimethylaminobenzaldehyde	Chloroform	4.02	266.5 °C	57.5 °C



<http://usefulchem.wikispaces.com/Exp209>



Conc Avg (M)	Conc. Std.Dev.
3.60	0.02

The Log makes Assumptions Explicit

Log

2008-09-30

11:00 Preweighed 60 half dram vials and labeled them 1b-60b.

12:00 Labeled 60 one dram vials in numerical order 1a-50a. *is the correct number 50 or 60 JCB*

12:15 Charged each vial with number specific solvent (listed in the spreadsheet)

12:30 Charged each vial with specific aldehyde, vortexed each for 30s. If solution was clear more sample was added until solution was saturated.

13:15 Skipped over samples 12, 22, 32, 42, 52 since not enough reagent was available.

13:35 4th row was skipped, not enough reagent.

15:25 Samples were finished with saturation step.

2008-10-02

12:30 Solvent was added to appropriate vials from which solvent had evaporated- All the vials had been capped tight (flip top) (- *next time get pic at this stage*)

13:20 Samples were vortexed again, until no more of the solid would dissolve..the vortex time varied from few seconds to about 7min, exact duration of vortex not recorded.

13:55 Samples were centrifuged.

13:57 Sample cracked in centrifuge; these solutions were remade in different vials and centrifuged carefully..

14:30 Then 300uL of the supernatant from each vial was carefully transferred to a corresponding half dram vial.

15:00 The vials with clear solutions (300uL each) were weighed.

16:00 The vials were capped after they were weighed.

2008-10-03

09:30 Placed the half dram in the speed-vac.

15:30 Removed the vials from the speed-vac.

16:00 Weighed the vials.

2008-10-07

11:00 Obtained pictures of the vials (one dram vials a-series, and the half dram vials b-series, which were left capped).



The Rationale of Findings Explicit

Discussion

The values for 4-chlorobenzaldehyde are very low in all solvents, including chloroform.--[HNMR](#) This is due to the prolonged time left in the speed-vac and the volatility of this aldehyde. Boiling point of 4-chlorobenzaldehyde at 1 atm. is 213-215 C ([Chemspider](#)) and the boiling point at 0.1 Torr is calculated to be 19 C (using a [reduced press. b.p calculator](#)). Since the pressure of the Speed-Vac can reach 0.05-0.1 Torr and the evaporation lasted 6 hours the solubility measurements for 4-chlorobenzaldehyde are not valid. The b.p of 2,6-dichlorobenzaldehyde at 1atm is 239.2 °C ([Chemspider prediction](#)), however saturated solutions of this compound in different solvents showed a concentration range between 0.42 M-3.41 M. This may indicate that only a very small amount of dry 2,6-dichlorobenzaldehyde may have evaporated, if at all. A similar trend is also seen with respect to 4-hydroxy benzaldehyde. Therefore the solubility values obtained for these compounds (but not 4-chlorobenzaldehyde) may still be used.

The densities for each solvent were determined by charging a small vial with 300ul of the solvent and measuring the differences in weight.

Methanol, chloroform, and THF did contain some error (*quantify*) from the literature value. The experimental values are in the [spreadsheet](#).

Conclusion

The solubilities of ten aldehydes were obtained in different solvents. Compounds with boiling points under 250C at 1 atm may not give valid solubility measurements when using the SpeedVac technique for several hours at about 0.1 Torr. Certainly for 4-chlorobenzaldehyde (b.p. 214C @ 1 atm) the measurement is unusable.

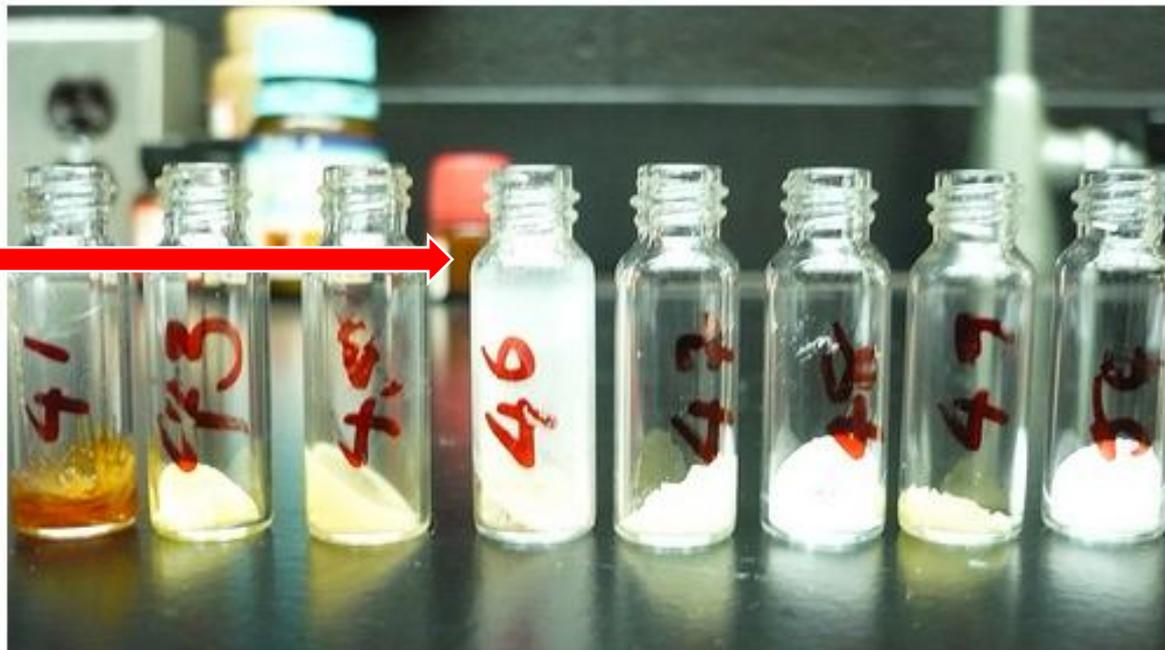


Raw Data Made Public

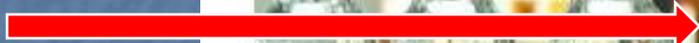


Usefulchem EXP208 41b-50b

ALL SIZES



Splatter?



Some liquid



Comments



[Chris Bohinski](#) pro says:

Hi, I'm an admin for a group called [Flickr Envy -- LOVE TO SHARE PHOTOS](#), and we'd love to have this added to the group!

Posted 5 weeks ago. ([permalink](#))

YouTube for demonstrating experimental set-up

Exp 009



0:17 / 0:35



Rate: ★★☆☆☆ 15 ratings

Views: 5,631

Calculations Made Public on Google Spreadsheets

EXP208-WS1

EXP208-WS1													
File Edit Format Insert Tools Form Help													
	A	B	C	D	E	F	G	H	I	J	K	L	M
	Si	ID	Solute	Solvent	Wt of empty vials (g)	Wt of vial w/solution (300uL)	Wt of sample solution (300uL)	Wt of vial after SpeedVac (g)	Solid dissolved in 300 uL of solvent (mg)	molecular weight of solid	Amt dissolved in 300 uL solvent (mmol)	Saturated Soln Conc (M)	Saturated soln-Density
2	1	1b	3,4-dimethoxyb	THF	2.57997	2.89851	0.31854	2.8292	249.23	166.17	1.50	5.00	1.0618
3	2	2b	3,5-dimethoxyb	THF	2.56974	2.8651	0.29536	2.77057	200.83	166.17	1.21	4.03	0.9845
4	3	3b	0-vanillin	THF	2.58903	2.92017	0.33114	2.83427	245.24	152.15	1.61	5.37	1.1038
5	4	4b	4-nitrobenzaldh	THF	2.56176	Aborted	Aborted	Aborted	Aborted	151.12	Aborted	Aborted	Aborted
6	5	5b	p-Toluenesulfon isocyanide	THF	2.54702	2.7989	0.25188	2.65069	103.67	186.21	0.56	1.86	0.8396



Revision History on Google Spreadsheets

Insert Tools Form Help

1 week(s) ago - tbjb27 - Began edits « Older Newer » Revert to this one Changed cells are highlighted

	molecular weight of solid	Amt dissolved in 300 uL solvent (mmol)	Saturated Soln Conc (M)	Saturated soln-Density	BP(predicted from ChemSpid at 760mmHg)
1 week(s) ago - tbjb27 - Began edits	166.17	1.50	5.00	1.0618	281 °C
1 week(s) ago - jeanclaude.bradley - Began edits	166.17	1.21	4.03	0.9845	276.5 °C
1 week(s) ago - tbjb27 - Began edits	152.15	1.61	5.37	1.1038	265.5 °C
2 week(s) ago - Khalidsmirza - Began edits	151.12	Aborted	Aborted	Aborted	299.6 °C
2 week(s) ago - Khalidsmirza - Began edits	186.21	0.56	1.86	0.8396	Unknown
2 week(s) ago - Khalidsmirza - Sorted					
2 week(s) ago - Khalidsmirza - Began edits					
3 week(s) ago - jeanclaude.bradley - Sorted					
3 week(s) ago - jeanclaude.bradley - Began edits					
3 week(s) ago - Khalidsmirza - Sorted					
3 week(s) ago - Khalidsmirza - Made edits					
3 week(s) ago - Khalidsmirza - Made edits					
3 week(s) ago - Khalidsmirza - Made edits					

Wiki Page History

 **UsefulChem**  **EXP208** page ▾ discussion **history**

Actions

-  [New Page](#)
-  [Recent Changes](#)
-  [Manage Space](#)



Navigation

- [All Experiments](#)
- [UC blog](#)
- [ONSchallenge](#)
- [UC on ChemSpider](#)
- [Mailing List](#)
- [Libraries](#)
- [References](#)
- [Experiment Format](#)

Date	Compare	Author
Nov 11, 2008 8:25 am	<input type="button" value="select"/>	 jcbradley
Nov 4, 2008 2:20 pm	<input type="button" value="select"/>	 khalidmirza
Oct 26, 2008 1:56 pm	<input type="button" value="select"/>	 jcbradley
Oct 23, 2008 6:39 am	<input type="button" value="select"/>	 jcbradley
Oct 21, 2008 12:41 pm	<input type="button" value="select"/>	 khalidmirza
Oct 21, 2008 12:31 pm	<input type="button" value="select"/>	 khalidmirza
Oct 21, 2008 10:24 am	<input type="button" value="select"/>	 jcbradley
Oct 20, 2008 6:19 pm	<input type="button" value="select"/>	 khalidmirza
Oct 20, 2008 3:51 pm	<input type="button" value="select"/>	 khalidmirza
Oct 20, 2008 3:41 pm	<input type="button" value="select"/>	 khalidmirza

Comparing Wiki Page Versions

Discussion

The values for 4-chlorobenzaldehyde are very low in all solvents, including chloroform.-- [HNMR](#) ↗ This is due to the prolonged time left in the speed-vac and the volatility of this aldehyde. Boiling point of 4-chlorobenzaldehyde at 1 atm. is 213-215 C ([Chemspider](#) ↗) and the boiling point at 0.1 Torr is calculated to be 19 C (using a [reduced press. b.p calculator](#) ↗). Since the pressure of the Speed-Vac can reach 0.05-0.1 Torr and the evaporation lasted 6 hours the solubility measurements for 4-chlorobenzaldehyde are not valid. [The b.p of 2,6-dichlorobenzaldehyde at 1atm is 239.2 °C \(\[Are there any other solutes\]\(#\) ↗ \[Chemspider prediction\]\(#\) \)](#), however saturated solutions of this compound in different solvents showed a concentration range between 0.42 M-3.41 M. This may indicate that only a very small amount of dry 2,6-dichlorobenzaldehyde may have evaporated, if at all. A similar trend is also seen with [low boiling points that might respect to 4-hydroxy benzaldehyde](#). Therefore the solubility values obtained for these compounds (but not 4-chlorobenzaldehyde) may still be [in error? used](#).

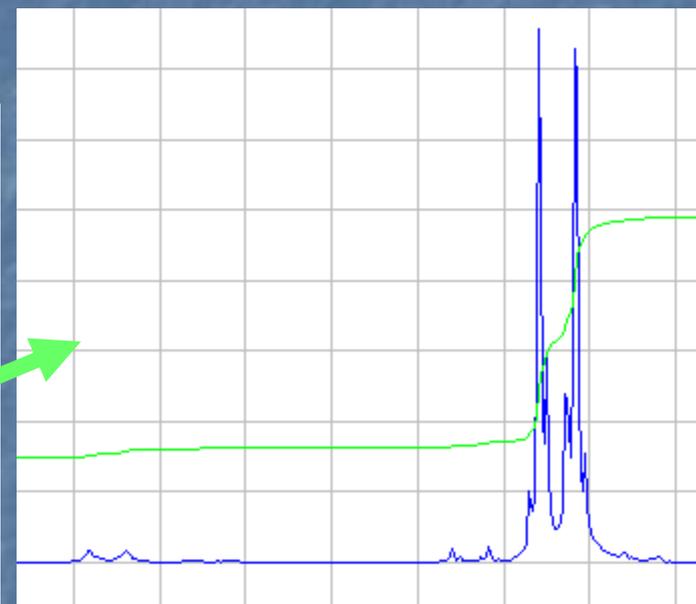
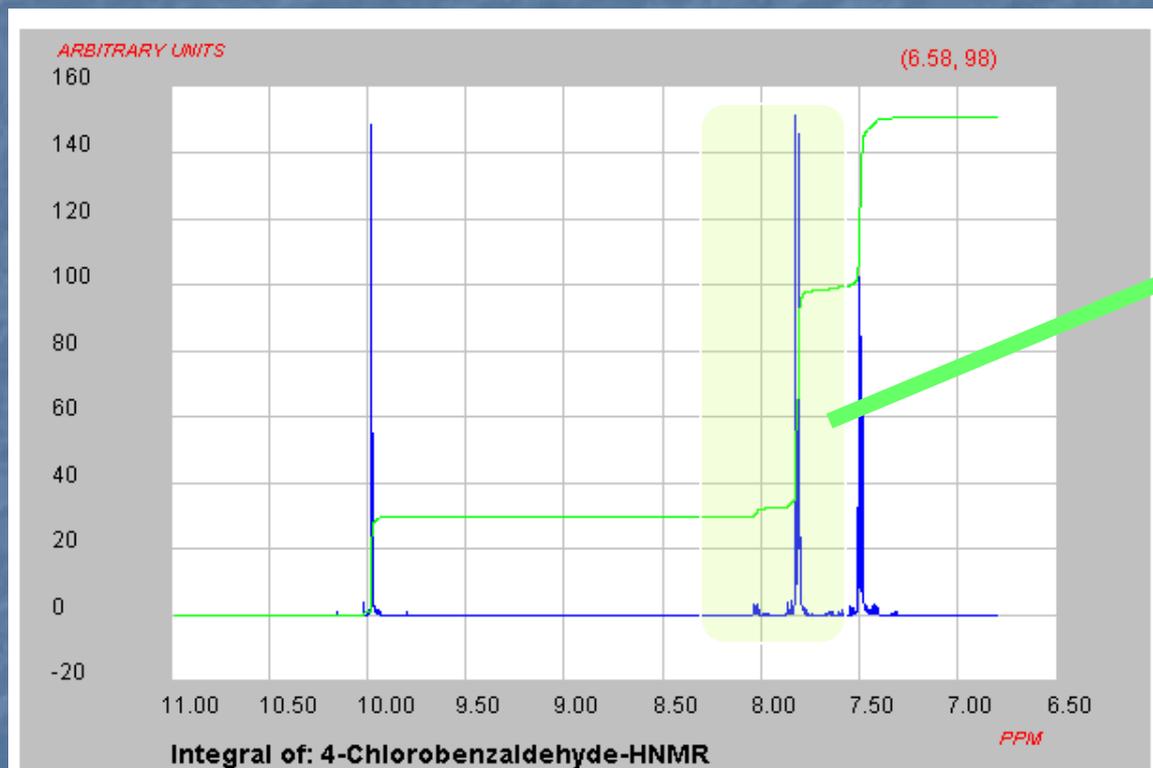
The densities for each solvent were determined by charging a small vial with 300ul of the solvent and measuring the differences in weight.

Methanol, chloroform, and THF did contain some error (*quantify*) from the literature value. The experimental values are in the [spreadsheet](#) ↗.

Conclusion

[Solubility of ten compounds were compounds were obtained in different solvents.](#)

Proof of Purity with interactive NMR spectrum using JSpecView and JCAMP-DX



JSpecView version number is 1.0.20071009-2130

Created and maintained by Prof Robert John Lancashire



<http://usefulchem.wikispaces.com/Exp208>

Indexing Molecules on Google

Tags

Compound	Inchikey	Inchi
Toluene	YXFVVABEGXRONW-UHFFFAOYAT	InChI=1/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
Acetonitrile	WEVYAHXRMPXWCK-UHFFFAOYAJ	InChI=1/C2H3N/c1-2-3/h1H3
Chloroform	HEDRZPFGACZZDS-UHFFFAOYAG	InChI=1/CHCl3/c2-1(3)4/h1H
Ethanol	LFQSCWFLJHTTHZ-UHFFFAOYAB	InChI=1/C2H6O/c1-2-3/h3H,2H2,1H3
Tetrahydrofuran	WYURNTSHIVDZCO-UHFFFAOYAI	InChI=1/C4H8O/c1-2-4-5-3-1/h1-4H2
3,4-dimethoxybenzaldehyde	WJUFSZVCOTFON-UHFFFAOYAT	InChI=1/C9H10O3/c1-11-8-4-3-7(6-10)5-9(8)12-2/h3-6H,1-2H3
o-vanillin	JJVNINGBHGBWJH-UHFFFAOYAB	InChI=1/C8H8O3/c1-11-7-4-2-3-6(5-9)8(7)10/h2-5,10H,1H3

[UsefulChem » EXP208 » code](#)

... [[<http://www.google.com/search?q=JJVNINGBHGBWJH|JJVNINGBHGBWJH>]]-[[<http://www.google.com/search?q=JJVNINGBHGBWJH-UHFFFAOYAB|UHFFFAOYAB>]] ...
[usefulchem.wikispaces.com/page/code/EXP208](#) - 28k - [Cached](#) - [Similar pages](#)

[UsefulChem » EXP208](#)

[JJVNINGBHGBWJH-UHFFFAOYAB](#) · [InChI=1/C8H8O3/c1-11-7-4-2-3-6\(5-9\)8\(7\)10/h2-5,10H,1H3](#) · 4-nitrobenzaldehyde · [BXRQSNOROATLV-UHFFFAOYAO](#) ...
[usefulchem.wikispaces.com/EXP208](#) - 123k - [Cached](#) - [Similar pages](#)
[More results from usefulchem.wikispaces.com »](#)

[o-Vanilline](#)

Registries: ChemSpider: [InChIKey=JJVNINGBHGBWJH-UHFFFAOYAB](#) · PubChem CID 8991 · PubChem ID 152156 · Google. Web, [sci-toys.com](#).
[sci-toys.com/scichem/jqp064/8991.html](#) - 14k - [Cached](#) - [Similar pages](#)

[Compounds from Journal: Synthesis - page 84](#)

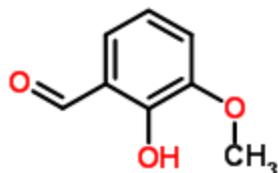
[JJVNINGBHGBWJH-UHFFFAOYAB](#). (3-bromophenyl)(phenyl)methanol. Molecular Formula: C₁₃H₁₁BrO. (3-bromophenyl)(phenyl)methanol. Molecular Weight: 263.134 g/mol ...
[www.chemsynthesis.com/journals/synthesis/page-84.html](#) - 47k - [Cached](#) - [Similar pages](#)

Linking to Molecules in Chemistry Databases



INHERENT PROPERTIES, IDENTIFIERS AND REFERENCES

2D 3D



ChemSpider ID: [21105848](#)
Empirical Formula: $C_8H_8O_3$
Molecular Weight: 152.1473
Nominal Mass: 152 Da
Average Mass: 152.1473 Da
Monoisotopic Mass: 152.047344 Da

load save zoom

Systematic Name: 2-hydroxy-3-methoxy-benzaldehyde

SMILES: Oc1c(ccc1OC)C=O

InChI: InChI=1/C8H8O3/c1-11-7-4-2-3-6(5-9)8(7)10/h2-5,10H,1H3

InChIKey: JJVNINGBHGWBWJH-UHFFFAOYAB

NAMES AND SYNONYMS

Validated by Experts, Validated by Users, r

205-715-3 [EINECS/ELINCS]

2-hydroxy-3-(methoxy)benzaldehyde

2-Hydroxy-m-anisaldehyde

Benzaldehyde, 2-hydroxy-3-methoxy-

ortho-vanillin

o-Vanillin

WIKIPEDIA ARTICLE(S)

Ortho-vanillin, 3-methoxysalicylaldehyde, is an essential oil of many plants. Its functional group, $C_8H_8O_3$, is distinctly different from its more common **hydroxy** moiety, which is found in the *para*-

SUPPLEMENTAL INFORMATION

User Data

- Experimental Physchem Properties

Melting Point: 40-42 

 **Melting Point:** 40 - 42 C  

Boiling Point: 265-266 

 **Boiling Point:** 265 C  

ASSOCIATED DATA SOURCES AND COMMERCIAL SUPPLIERS

Data Source	
Alfa Aesar 	A15672
ASDI 	500011405
ChemPacific 	 PREDICTED PROPERTIES

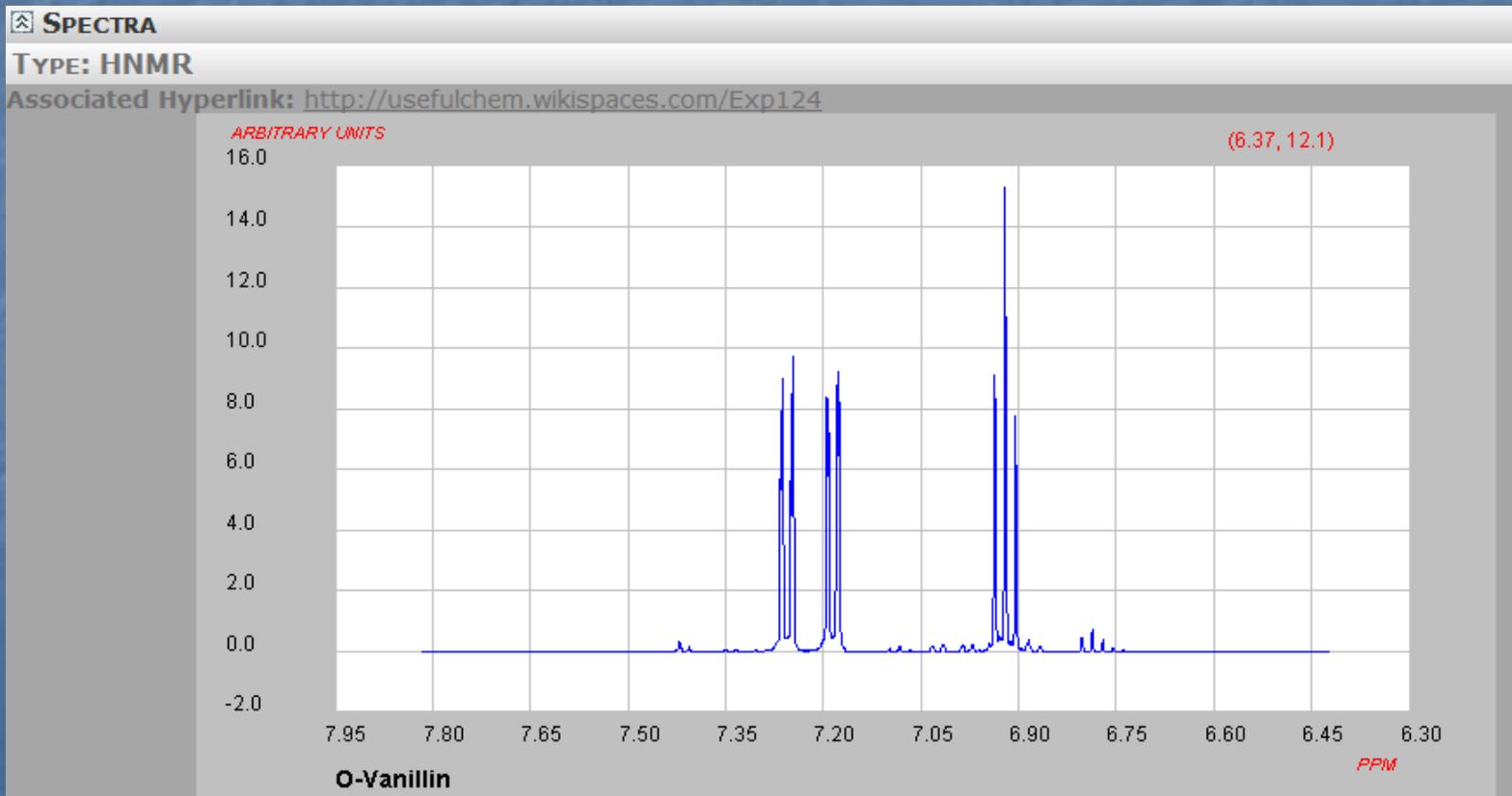
Boiling Point: 265.5 °C at 760 mmHg

Experimental Spectra and User-Deposited Data on ChemSpider

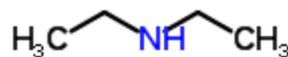
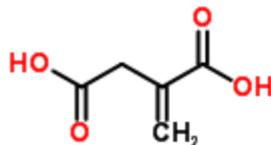
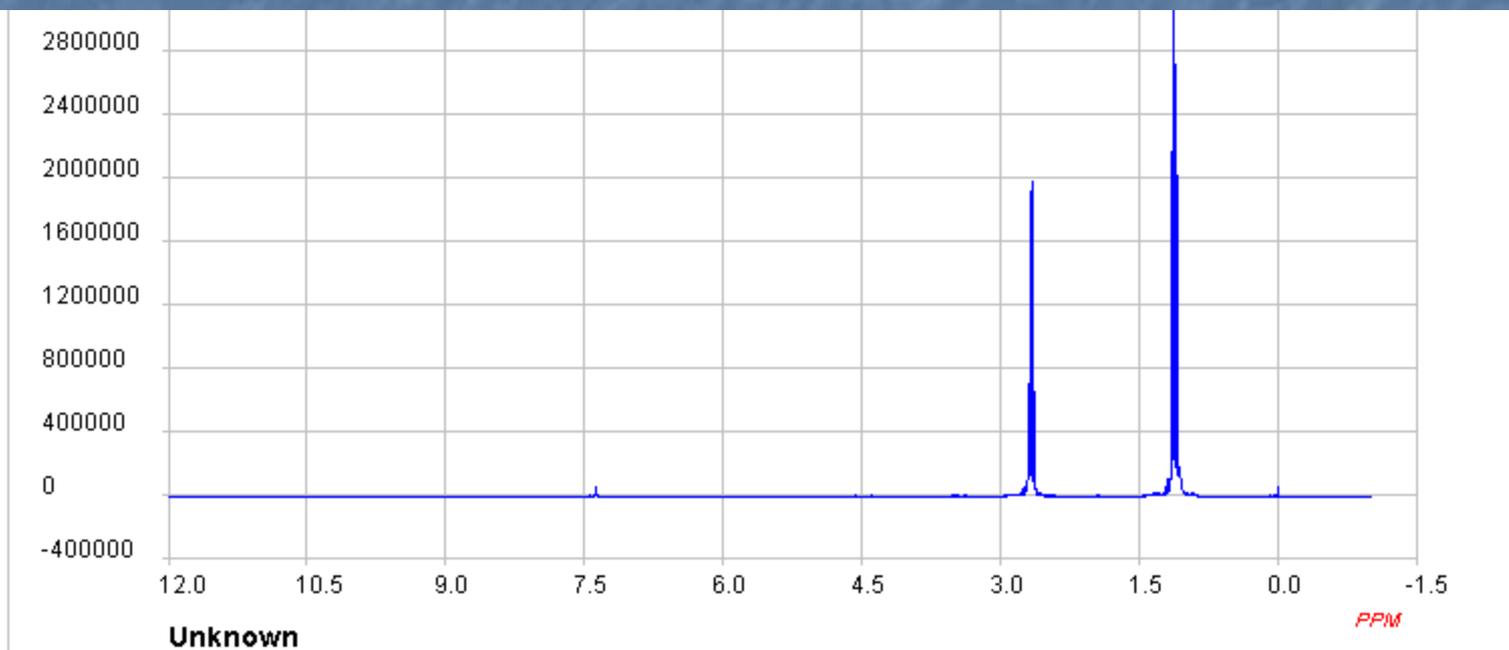
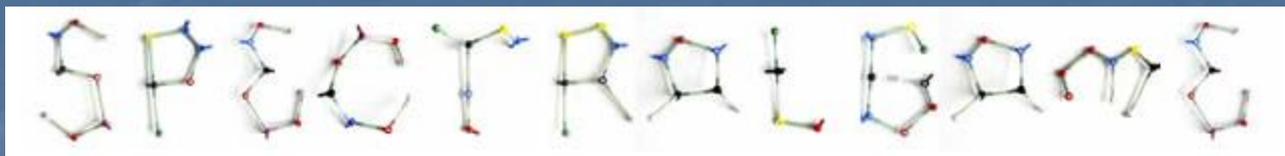
SUPPLEMENTAL INFORMATION

User Data

- Experimental Physchem Properties**
Non-Aqueous Solubility: 1.32M in methanol  



Open Data JCAMP spectra for education



Database Curation via Game Playing

Click on the molecule that corresponds to the spectrum. Hit F11 to enlarge browser window.

No spectrum? Spectrum reversed? **FLAG IT!**

No spectrum? Something wrong with the spectrum? **Comment.** (opens in new window)



Over 50,000 spectrum views so far -
worldwide

Top Scores			
Player	Group	Type	Score
milkshake	N. Voss of Berlin	HNMR	51
SiO2lungs	REM	HNMR	43
milkshake	N/A	HNMR	42
anon	N/A	HNMR	41
VK	N/A	HNMR	40
lastpook	bsu	HNMR	40
milkshake	N/A	HNMR	40
milkshake	N/A	HNMR	40
joko	mz	HNMR	40
Johannes	uhh	HNMR	39
milkshake	N/A	HNMR	39
sniecker	N/A	HNMR	37
lastpook	bsu	HNMR	37
milkshake	N/A	HNMR	37
top	uhh	HNMR	37
milkshake	N/A	HNMR	37
milkshake	N/A	HNMR	37
GAWD	N/A	HNMR	36
SiO2lungs	REM	HNMR	36

Link Spectral Game to Open Educational Content

The Spectral Game

Developed by Jean-Claude Bradley, Robert Lancashire, Andrew Lang and Antony Williams

Links

[Play the game!](#)

[Latest and High Scores](#)

[Contribute spectra](#) to [ChemSpider](#) as Open Data.

[UsefulChem 3/1/09 post](#)

Spectroscopy Resources

[Organic Structure Determination \(Open Courseware\)](#)

[WebSpectra](#)

[Spectroscopy Page](#) (Organic Chemistry Wikibook)

The following taken from [Organic Chemistry II at Drexel University](#) taught by Jean-Claude Bradley:

Nuclear Magnetic Resonance Spectroscopy (NMR)

- [Reusch](#)
- can view every H and C in molecules as peaks
- scale in ppm (delta scale), relative to tetramethylsilane (TMS), defined as zero
- in a typical NMR plot, higher ppm are on the left (low field, more deshielded)
- integration corresponds to number of Hs

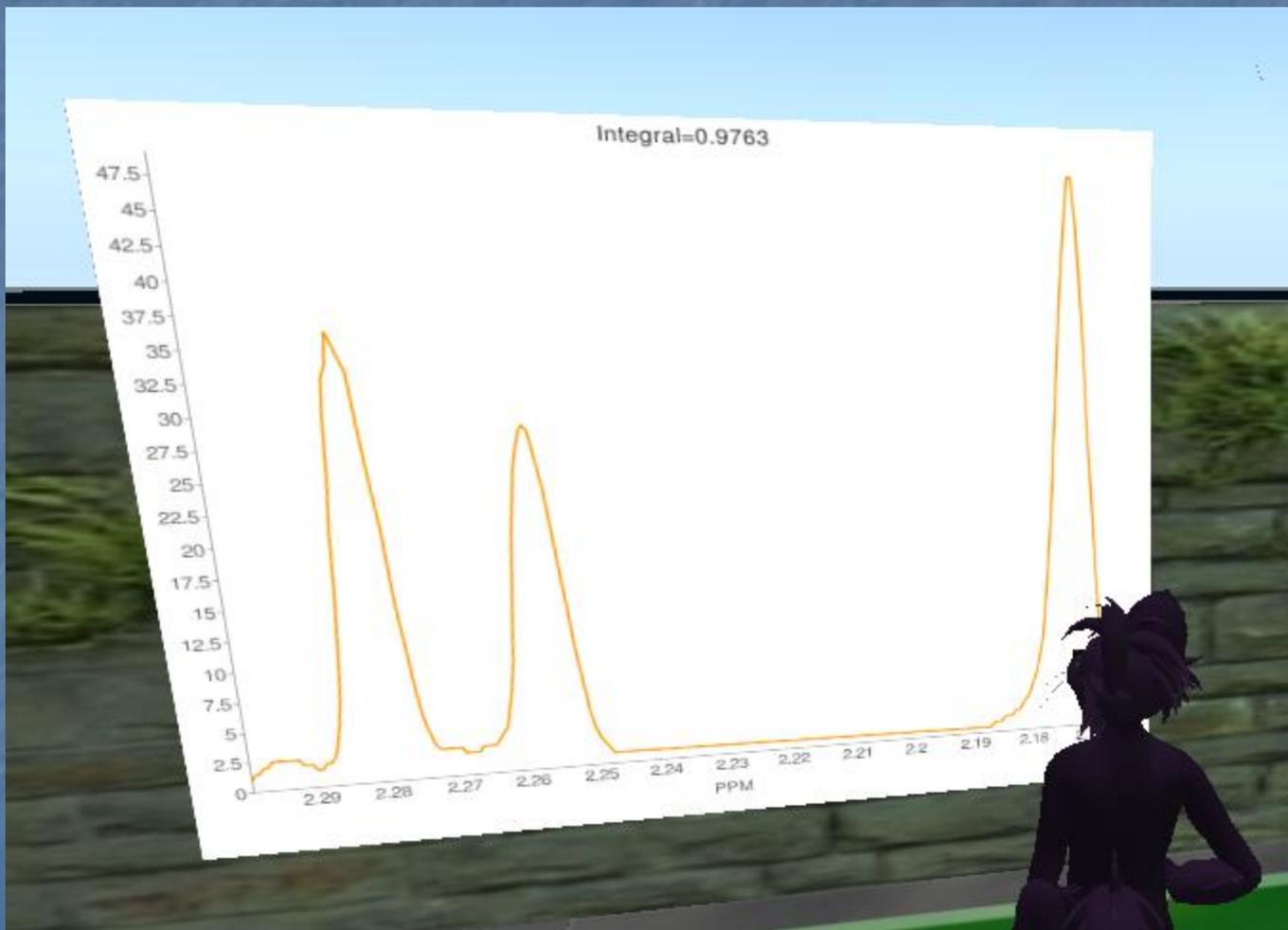
<http://spectralgame.wikispaces.com/>

Prizes not Punishment to motivate students

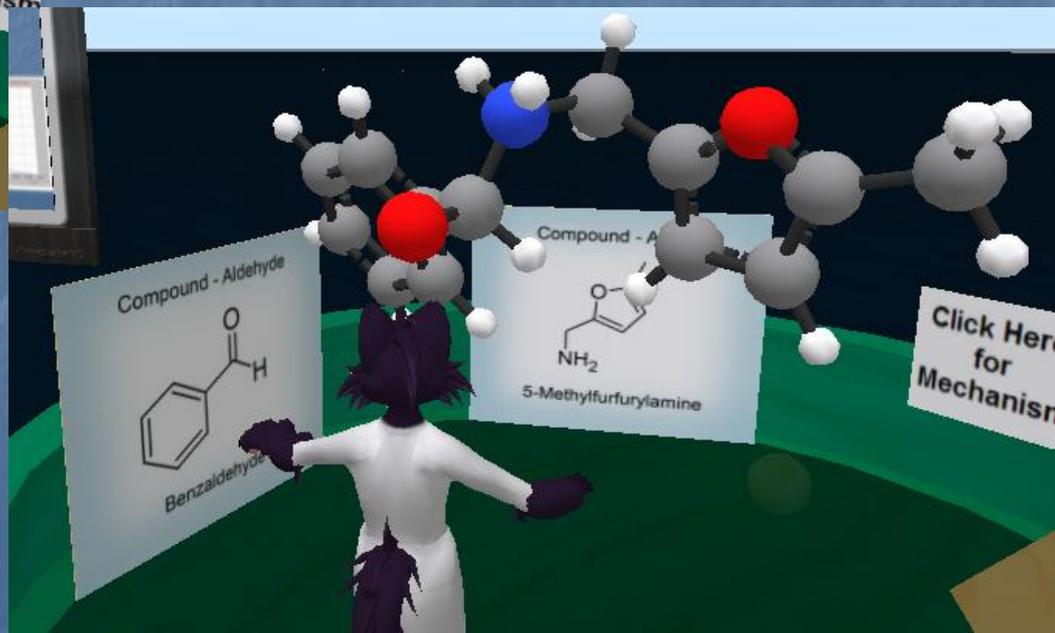
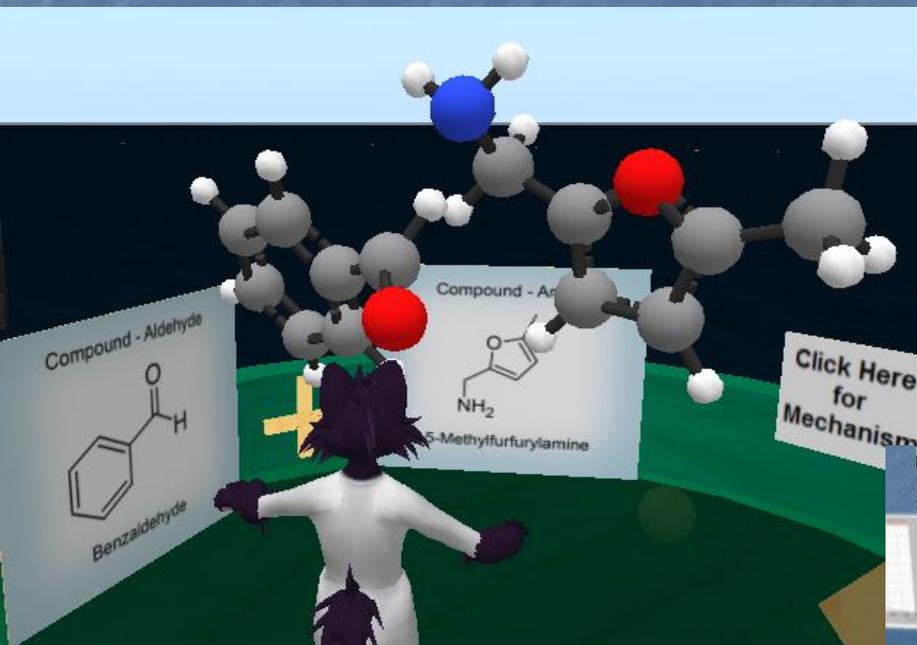
Top Scores			
Player	Group	Type	Score
Adrian	Drexel	all	17
Adrian	Drexel	all	15
Fox	Drexel	all	13
Adrian	Drexel	all	4
Adrian	Drexel	all	4
ashlie glasgow	drexel	all	2
Adrian	Drexel	all	1
Adrian	Drexel	all	1
Adrian	Drexel	all	1
Adrian	Drexel	all	0
Adrian	Drexel	all	0
Adrian	Drexel	all	0

Lastest Scores			
Player	Group	Type	Score
Mario	N/A	all	3
Tony	N/A	lewisstructure	2
ashlie glasgow	drexel	all	2
drb	N/A	hybridization	80
drb	N/A	all	3
drb	N/A	all	4
Bibi	N/A	nomenclature	2
chiral	N/A	chirality	1
chiral	N/A	chirality	0
Gianni	N/A	all	11
Adrian	Drexel	all	17
free radical?	N/A	freeradical	2
Adrian	Drexel	all	4
Adrian	Drexel	all	15
test	N/A	newman	9
test	N/A	hybridization	3
mch	N/A	all	2
mch	N/A	all	1

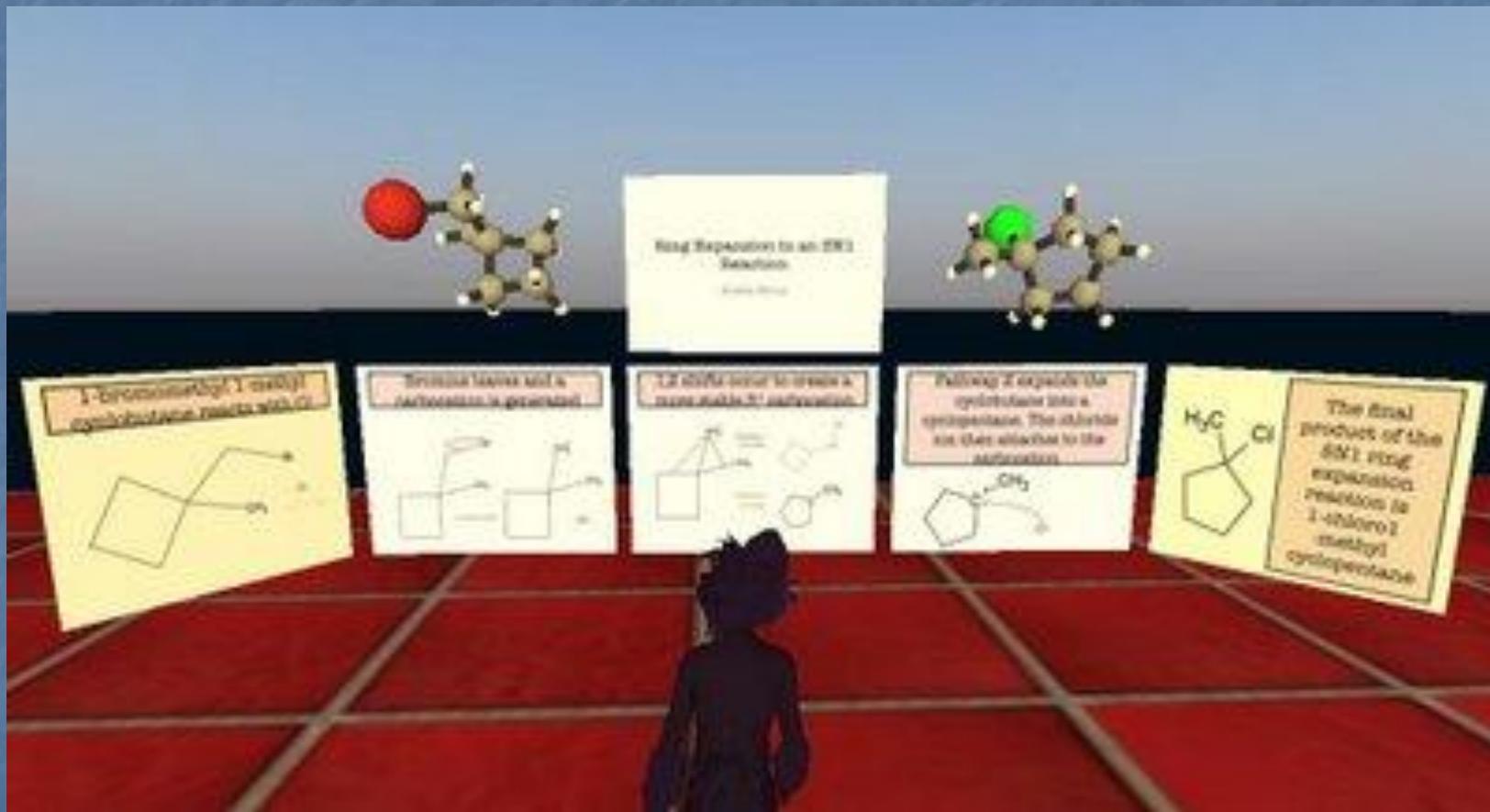
Talk to the spectrum: zoom 2.1-2.3 (Andy Lang)



Imine Formation Mechanism: talk to the molecules!



Student Projects in Second Life



Spring 09 projects: networking in Second Life and FriendFeed

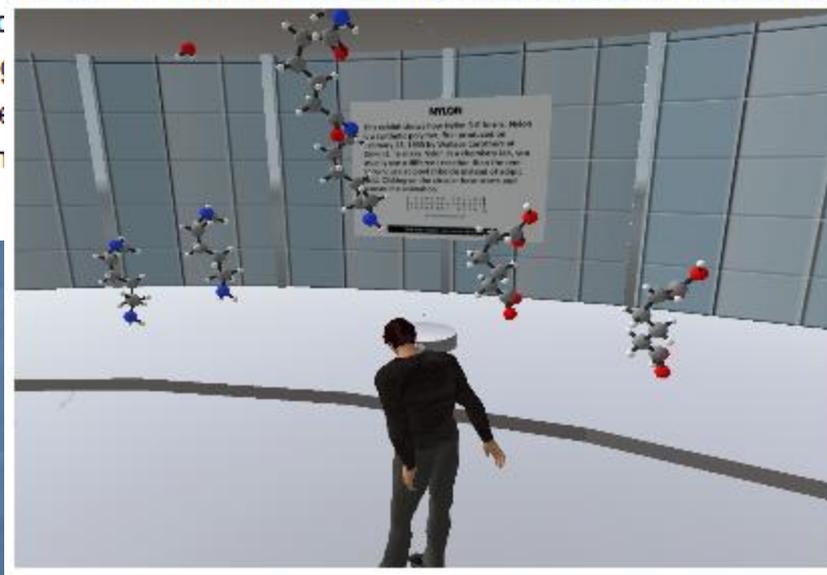
Second Life Interviews (Second Life Names)

Arij Pevensey is a student (majoring in chemistry for three years now) who is interested in molecular models and chemical data visualizations.

Georgianna Blackburn is an e-marketer (for Sigma Aldrich for two years) who joined Second Life in order to investigate new technologies for product delivery and joined Second Life in order to investigate new technologies for product delivery.

Hiro Sheridan is a professor (of mathematics @ ORU and has been interested in multi-dimensional chemical data visualization and joined Second Life in order to investigate new technologies for product delivery and chemical data visualizations in Second Life).

Nylon polymerization ([http://slurl.com/secondlife/AC S/176/239/25](http://slurl.com/secondlife/AC%20S/176/239/25))



<http://chem241.wikispaces.com/extracredit>

Crowdsourcing Solubility Data

Open Notebook Science Challenge

Sponsors



[Submeta Open Notebook Science Awards - Apply Here](#)

What?

The first round of this challenge calls upon people with access to materials and equipment to measure the solubility of compounds (aldehydes, amines and carboxylic acids are a priority) in organic solvents and report their findings using [Open Notebook Science](#) . (see [cumulative list of results here](#)  or in [RDF format](#) )



<http://onschallenge.wikispaces.com/>

ONS Challenge Students

Students

Jenny Hale (December 2008 Submeta Award winner)

Supervisor: Cameron Neylon

Age: 26

Location: University of Southampton, England

Education: BSc Chemistry with pharmacology, 200

Currently PhD student Investigating directed evoluti

Cedric Tchakounte (March 2009 Submeta Award winner)

Supervisor: Jean-Claude Bradley

Location: Drexel University, Philadelphia

Education: Jr. at Drexel University

Major: Biological Sciences & Biotechnology

Khalid Mirza (January 2009 Submeta A

Supervisor: Jean-Claude Bradley

Location: Drexel University, Philadelphia

Currently PhD student Investigating the synthesis c

Tim Bohinski (April 2009 Submeta Award winner)

Supervisor: Jean-Claude Bradley

Age:21

Location: Drexel University, Philadelphia

Education: Jr. at Drexel University

Major- Chemistry

Employer- Johnson Matthey Catalyst and Precious Metal Refinery Analytical Lab,

David Bulger (February 2009 Submeta

Supervisor: Robert Stewart

Age:19

Location: Oral Roberts University

Education: So. at Oral Roberts University

Major: Chemistry



ONS Challenge Judges

Submeta ONS Award judges

- [Jean-Claude Bradley](#) (Associate Professor of Chemistry at Drexel University)
- [Cameron Neylon](#)  (Senior Scientist at the ISIS Pulsed Neutron Source, Rutherford Appleton Laboratory, near Oxford with a joint appointment as a Lecturer in Chemical Biology at the School of Chemistry at the University of Southampton)
- [Rajarshi Guha](#)  (Visiting Professor at Indiana University)
- [Antony Williams](#)  (President of ChemZoo, NMR specialist)
- [Bill Hooker](#)  (postdoctoral researcher in molecular biology at Shriners Hospital for Children)



<http://onschallenge.wikispaces.com/judges>

Teaching Lab: Brent Friesen (Dominican University)

Tentative Laboratory Schedule: Spring 2009

Date	Title
1/21,22, 23	1) Solubility Challenge
1/28,29,30	2) Diels Alder
2/04,05,06	3) Essential Oils
2/11,12,13	4) Synthetic Azo Dyes

Solubility Experiment List

List of Experiments on this wiki

[Exp078](#) Determination of the solubility of one Ugi product in six solvents - **Matthew Federici**

[Exp077](#) Determination of the solubility of Diphenylacetic acid in methanol - **Matthew Federici**

[Exp076](#) Determination of the solubility of two Ugi products in six solvents - **Shuba, Khalid**

[Exp075](#) Determination of the solubility of 4-chlorophenylacetic acid in seven solvents - **Shuba, Khalid**

[Exp074](#) Determination of the solubility of 4-pyrenebutanoic acid in THF and a 3:1 mix of THF and methanol - **Khalid**

[Exp073](#) Determination of the solubility of 4-chlorophenylacetic acid in methanol and THF using 2 methodologies by NMR-
Cedric

[Exp072](#) Determination of the solubility of DL-mandelic acid, trans-cinnamic acid, 4-phenylbutyric acid, L-ascorbic acid, acetylsalicylic acid and 4,4-azoxydibenzoic acid in various solvents using ¹H NMR - **David**

[Exp071](#) Determination of the solubility of the Ugi product UC215C, vertatraldehyde, piperonal and Boc-glycine in different solvents - **Khalid**

[Exp070](#) Determination of the solubility of Octadecylamine and 5 solvents - **HaeJi**

[Exp069](#) Determination of the solubility of Octadecylamine and 5 solvents - **HaeJi**

[Exp068](#) Determination of the solubility of TOSMIC and octadecylamine in acetonitrile - **Khalid**



Summary of Solubility Experiments



Solvents

Displaying solvents that have more than three solute solubility values. Select the solvent to view the [chemical space](#).

Solvent	Solutes	aldehydes	amines	isonitriles	carboxylic acids	Ugi-products	Non-Ugi-related
methanol	103	35	10	0	39	14	5
ethanol	47	17	3	1	20	2	4
THF	38	17	2	1	12	3	3
acetonitrile	20	11	1	1	5	2	0
chloroform	20	9	0	1	9	1	0
toluene	17	9	1	1	4	2	0
DMSO	8	3	0	0	3	2	0
hexane	8	3	0	0	3	1	1
benzene	7	2	0	0	3	1	1
dichloromethane	7	4	0	0	2	1	0
diethyl ether	7	3	0	0	2	1	1
2-propanol	5	2	0	0	2	1	0
N,N-dimethylformamide	4	2	0	0	1	1	0
acetone	4	1	0	0	2	0	1
carbon tetrachloride	4	1	0	0	1	1	1
cyclohexane	4	2	0	0	1	1	0

Solubilities collected in a Google Spreadsheet

Google Docs BETA

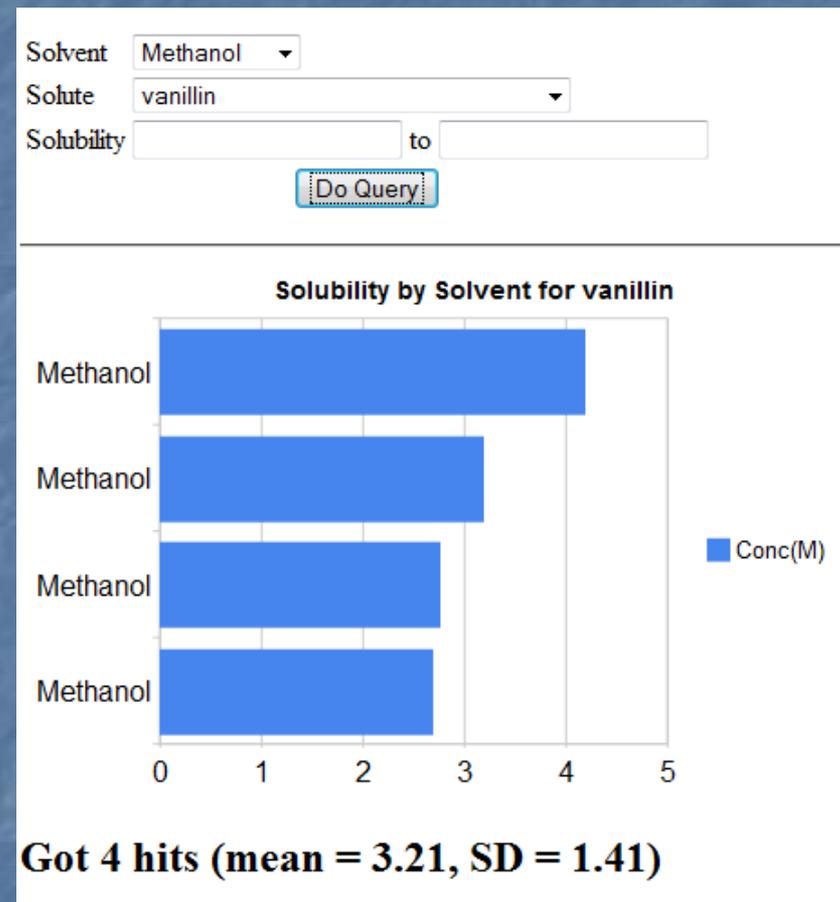
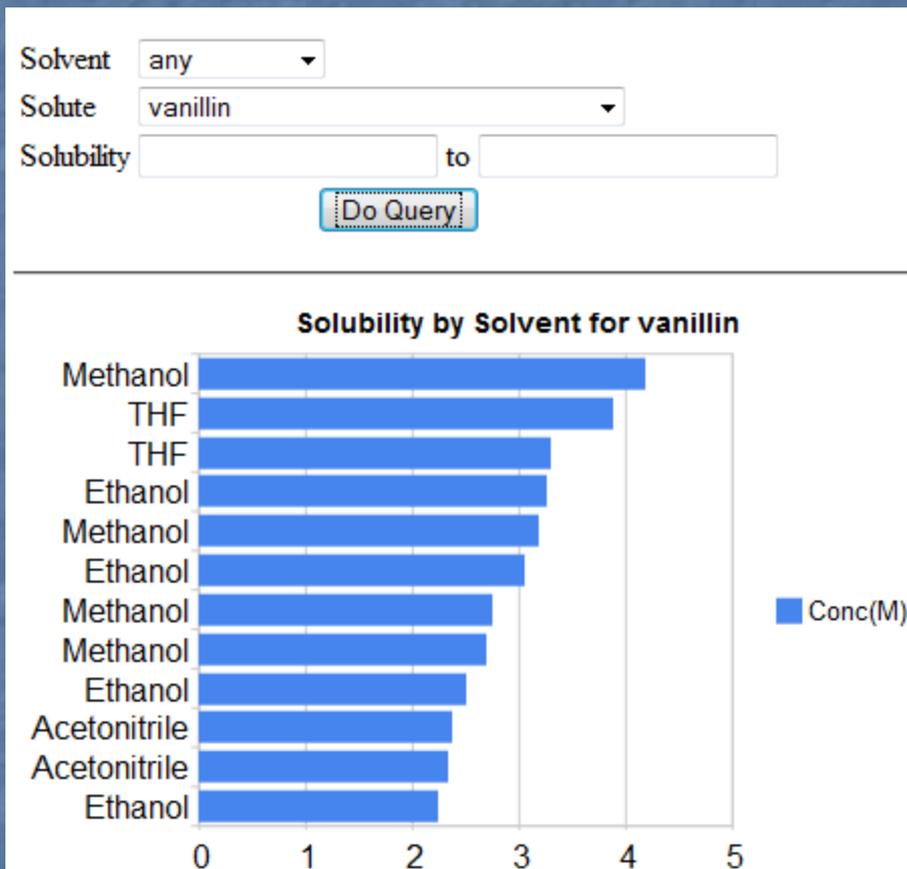
SolubilitiesSum

File Edit Format Insert Tools Form Help

	A	B	C	D
	EXP	sample	ref	solute
2	208	11b	http://usefulchem.wikispaces.com/exp208	3,4-dimethoxybenzaldehyde
3	208	41b	http://usefulchem.wikispaces.com/exp208	3,4-dimethoxybenzaldehyde
4	208	21b	http://usefulchem.wikispaces.com/exp208	3,4-dimethoxybenzaldehyde
5	208	3b	http://usefulchem.wikispaces.com/exp208	o-vanillin
6	208	1b	http://usefulchem.wikispaces.com/exp208	3,4-dimethoxybenzaldehyde
7	205	1	http://usefulchem.wikispaces.com/exp205	3,4-dimethoxybenzaldehyde
8	210	40	http://usefulchem.wikispaces.com/exp210	crotonic acid

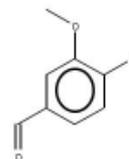
solute SMILES	solvent	solvent SMILES	concentration (M)	wiki page	Added to ChemSpider SDF
<chem>COc1cc(ccc1OC)C=O</chem>	Acetonitrile	<chem>N#CC</chem>	5.57	UC	
<chem>COc1cc(ccc1OC)C=O</chem>	Ethanol	<chem>OCC</chem>	5.55	UC	
<chem>COc1cc(ccc1OC)C=O</chem>	Chloroform	<chem>ClC(Cl)Cl</chem>	5.44	UC	
<chem>Oc1c(cccc1OC)C=O</chem>	THF	<chem>O1CCCC1</chem>	5.37	UC	
<chem>COc1cc(ccc1OC)C=O</chem>	THF	<chem>O1CCCC1</chem>	5.00	UC	
<chem>COc1cc(ccc1OC)C=O</chem>	Methanol	<chem>OC</chem>	4.92	UC	
<chem>O=C(O)/C=C/C</chem>	Ethanol	<chem>OCC</chem>	4.65	UC	
<chem>O=C(O)/C=C/C</chem>	Methanol	<chem>OC</chem>	4.56	UC	
<chem>O=C(OC(C)(C)C)NCC(=O)O</chem>	Methanol	<chem>OC</chem>	4.40	UC	YES
<chem>O=C(O)/C=C/C</chem>	Methanol	<chem>OC</chem>	4.2	UC	

Rajarshi Guha's Live Web Query using Google Viz API



Serial	EXP	Sample	Ref	Solute	Solute SMILES	Solvent	Solvent SMILES	Conc (M)
--------	-----	--------	-----	--------	---------------	---------	----------------	----------

1	207	3	http://usefulchem.wikispaces.com/exp207	vanillin	<chem>O=Cc1ccc(OC)c(O)c1</chem>	Methanol	OC	4.19
---	-----	---	---	----------	---------------------------------	----------	----	------



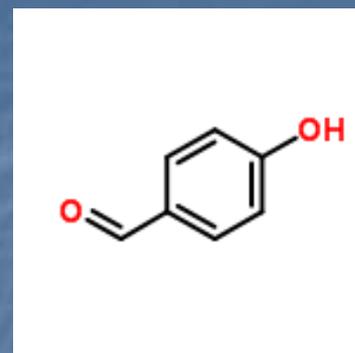
Substructure Searching of solubility data

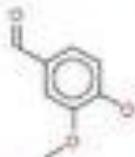
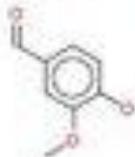
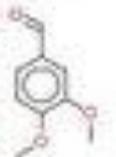
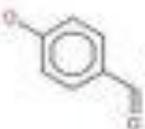
Solvent

Solute

Solubility to

SMARTS

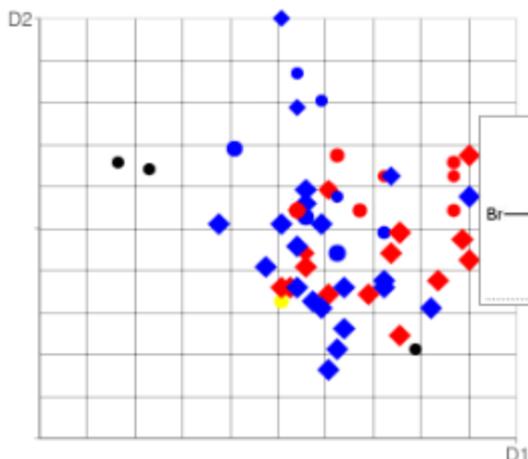


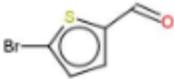
1	208	6b	http://en.wikipedia.org/wiki/4-hydroxybenzaldehyde	4-hydroxybenzaldehyde		<chem>O=Cc1ccc(O)cc1</chem>	THF	3.51
2	1	12-	http://en.wikipedia.org/wiki/3-methoxybenzaldehyde	vanillin		<chem>Oc1ccc(cc1OC)C=O</chem>	THF	3.298
3	207	15-	http://en.wikipedia.org/wiki/3-methoxybenzaldehyde	vanillin		<chem>Oc1ccc(cc1OC)C=O</chem>	THF	3.89
4	208	1b	http://en.wikipedia.org/wiki/3-methoxybenzaldehyde	vanillin		<chem>COc1cc(oc1OC)C=O</chem>	THF	5
5	57	7-	http://en.wikipedia.org/wiki/4-hydroxybenzaldehyde	4-hydroxybenzaldehyde		<chem>O=Cc1ccc(O)cc1</chem>	THF	0.909
6	57	10-	http://en.wikipedia.org/wiki/3-methoxybenzaldehyde	4-hydroxy-3-methoxybenzaldehyde		<chem>O=Cc1ccc(O)c(OC)c1</chem>	THF	3.052

Rajarshi Guha and Andy Lang: Chemical Space Explorer

OPEN
NOTEBOOK
SCIENCE

descriptor chemical space for methanol





Solute	5-bromothiophene-2-carbaldehyde
SMILES	<chem>C1=C(SC(=C1)Br)C=O</chem>
Concentration	9.22
Type	aldehyde

KEY: x-axis: ALOGP - y-axis: Weight

Pointsize is proportional to solubility value - Hover mouse over point to view data [Firefox].

● aldehyde

● amine

● carboxylic acid

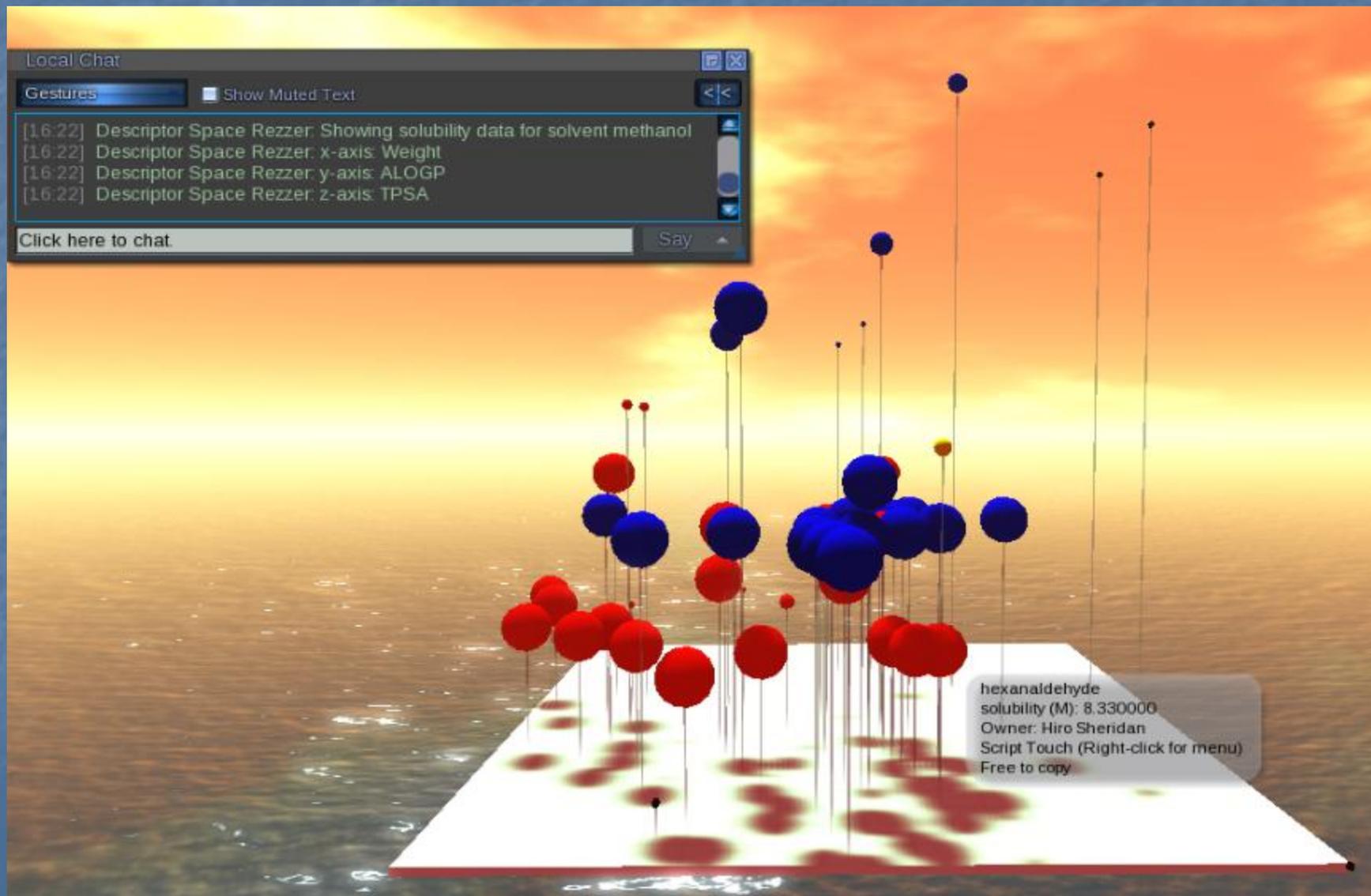
● isonitrile

● non UGI-related

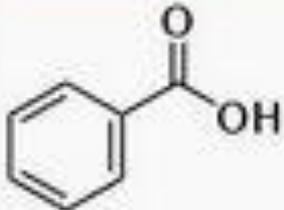
Number of Solutes: 59 - Click on the concentration value to see where the solubility data comes from.

Solute	Solute Smiles	Concentration (M)	Solute Type
2,2-diphenylacetaldehyde	<chem>C1=CC=C(C=C1)C(C=O)C2=CC=CC=C2</chem>	5.64	aldehyde
2,4-dimethylbenzaldehyde	<chem>CC1=CC(=C(C=C1)C=O)C</chem>	7.17	aldehyde

Andy Lang: Chemical Space Explorer in Second Life



From Wikipedia to...

Benzoic acid	
	

Properties	
Molecular formula	C ₆ H ₅ COOH
Molar mass	122.12 g/mol
Appearance	Colourless crystalline solid
Density	1.32 g/cm ³ , solid
Melting point	122.4 °C (395 K)
Boiling point	249 °C (522 K)
Solubility in water	Soluble (hot water) 3.4 g/l (25 °C)
Solubility in THF, ethanol, methanol	THF 3.646 M, ethanol 2.435 M, methanol 2.904 M ^[1]

References

- ¹ <http://oru.edu/ccoda/sl/solubility/allsolvents.php?solute=benzoic%20acid>  Open Notebook Science Challenge Data.

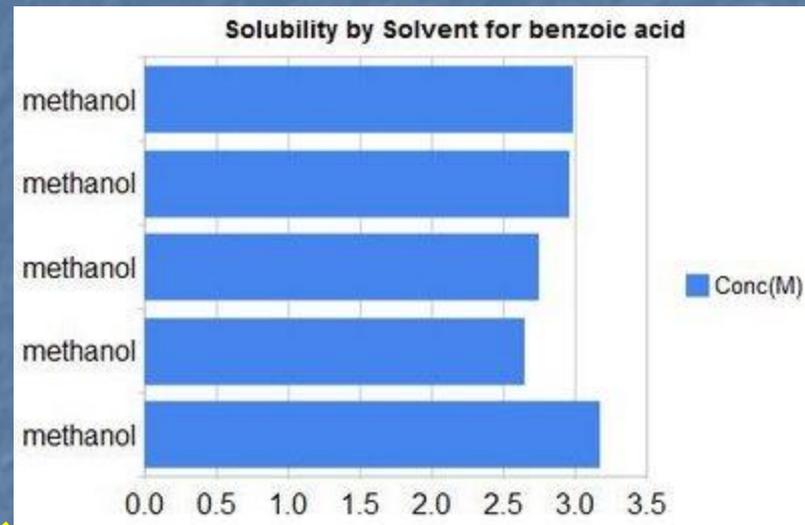


...the lab notebook and raw data

OPEN NOTEBOOK SCIENCE CHALLENGE

Solubility of benzoic acid in non-aqueous solvents.
 Total Number of Results: 13
 Total Number of Solvents: 5

Solvent	Hits	Mean Conc. (M)	SD	Link to Detailed Results
1. THF	2	3.646	0.073	Solubility of benzoic acid in THF
2. acetonitrile	2	0.757	0.015	Solubility of benzoic acid in acetonitrile
3. ethanol	2	2.435	0.002	Solubility of benzoic acid in ethanol
4. methanol	5	2.904	0.182	Solubility of benzoic acid in methanol
5. toluene	2	0.63	0	Solubility of benzoic acid in toluene



Exp005 Edit This Page page discussion history notify me

Objective
 To measure the solubility of benzoic acid ([Chemspider](#)), in methanol ([Chemspider](#)). For project see [here](#).

Procedure
 Saturated solutions are made of benzoic acid ([Chemspider](#)), in methanol ([Chemspider](#)) dram vial with 700µl of the solvent.
 The solute is then added in subsequent amounts until the solution has reached a clear point of saturation. Each vial is vortexed for 30 seconds. After the process of vortexing is complete, the solution is centrifuged for one minute. 300µl of the mother liquor is then pipetted into pre-weighed half-dram vials. The solution is weighed and entered into the speedvac, noting the pressure. The solution is then dried until the liquid has evaporated off. The results can be found on the following [Spreadsheet](#).

Solute	Solvent	Wt of empty vials (g)
Benzoic acid	Methanol	2.55842
Benzoic acid	Methanol	2.56923

Including links to the literature

OPEN
NOTEBOOK
SCIENCE
CHALLENGE

Solubility of benzoic acid in methanol
Number of Results: 5

Experiment Page or Citation	Solute	Solvent	Concentration (M)	Notes
1. http://onschallenge.wikispaces.com/Exp005	benzoic acid	methanol	2.9883	-
2. http://onschallenge.wikispaces.com/Exp005	benzoic acid	methanol	2.9572	-
3. http://onschallenge.wikispaces.com/Exp007	benzoic acid	methanol	2.7487	-
4. http://onschallenge.wikispaces.com/Exp007	benzoic acid	methanol	2.6561	-
5. Seidel, A. Solubilities of Inorganic and Organic Compounds (1919)	benzoic acid	methanol	3.17	23°C

n=5
mean=2.904
standard deviation=0.1823



135

BENZOIC ACID

SOLUBILITY OF BENZOIC ACID IN 90% ALCOHOL, IN ETHER AND IN CHLOROFORM. (Bourgoin.)

Solvent.	t°.	Gms. C ₆ H ₅ COOH per 100 Grams.	
		Solvent.	Solution.
90% Alcohol	15	41.62	29.39
Ether	15	31.35	23.86
Chloroform	25	14.30	12.50

SOLUBILITY OF BENZOIC ACID IN SEVERAL ALCOHOLS. (Timofiew, 1894.)

Alcohol.	t°.	Gms. C ₆ H ₅ COOH per 100 Gms.		Alcohol	t°.	Gms. C ₆ H ₅ COOH per 100 Gms.	
		Sat. Sol.	Solvent.			Sat. Sol.	Solvent.
Methyl	-18	23.1	30	Propyl	-18	14.5	16.9
"	-13	24.3	32.1	"	-13	15.7	18.5
"	+3	33.5	50.4	"	+3	23.1	30
"	19.2	40.1	67.1	"	19.2	28.2	39.3
"	23	41.7	71.5	"	23	29.8	42.3
Ethyl	-18	20.3	25.4	Isopropyl	21.2	32.7	48.5
"	-13	21.2	26.9	Allyl	21.2	25.1	33.4
"	+3	28.8	40.4	Isobutyl	0	15.3	18
"	19.2	34.4	52.4	Isoamyl	18	20.2	25.4
"	23	35.9	55.9	Caprylic	21.2	22.7	28.7
				Ethylene glycol	18	8	8.69

Additional data, agreeing closely with the above, are given by Timofiew (1891) and Bourgoin (1878).

Get Results from Mechanical Turk Workers

Ask workers to complete HITs - *Human Intelligence Tasks* - and get results using Mechanical Turk. [Get started.](#)

As a Mechanical Turk Requester you:

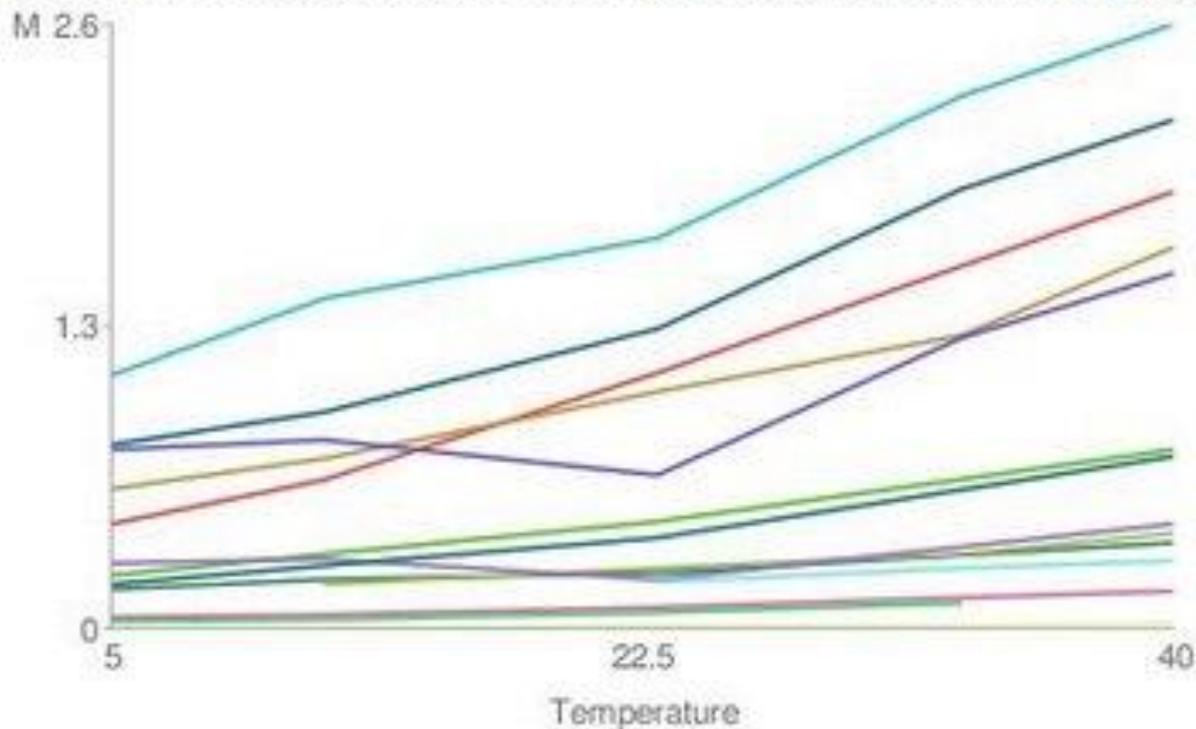
- Have access to a global, on-demand, 24 x 7 workforce
- Get thousands of HITs completed in minutes
- Pay only when you're satisfied with the results



<u>HIT Template Name</u>	<u>HIT Title</u>
Remove Capitals Solutes	Edit text to spreadsheet See an example
Follow Pattern	Add text to spreadsheet See an example
Remove Capitals Solvents	Edit text to spreadsheet See an example
Column SMILES add	Add text to spreadsheet See an example
Column format change	change text formatting See an example
Table Processing	Extract tabular data from image to spreadsheet See an example
sol2	Find solubility information See an example
sol1	Find solubility information See an example

Temperature info automatically plotted

The effect of temperature on the solubility of 4-nitrobenzaldehyde

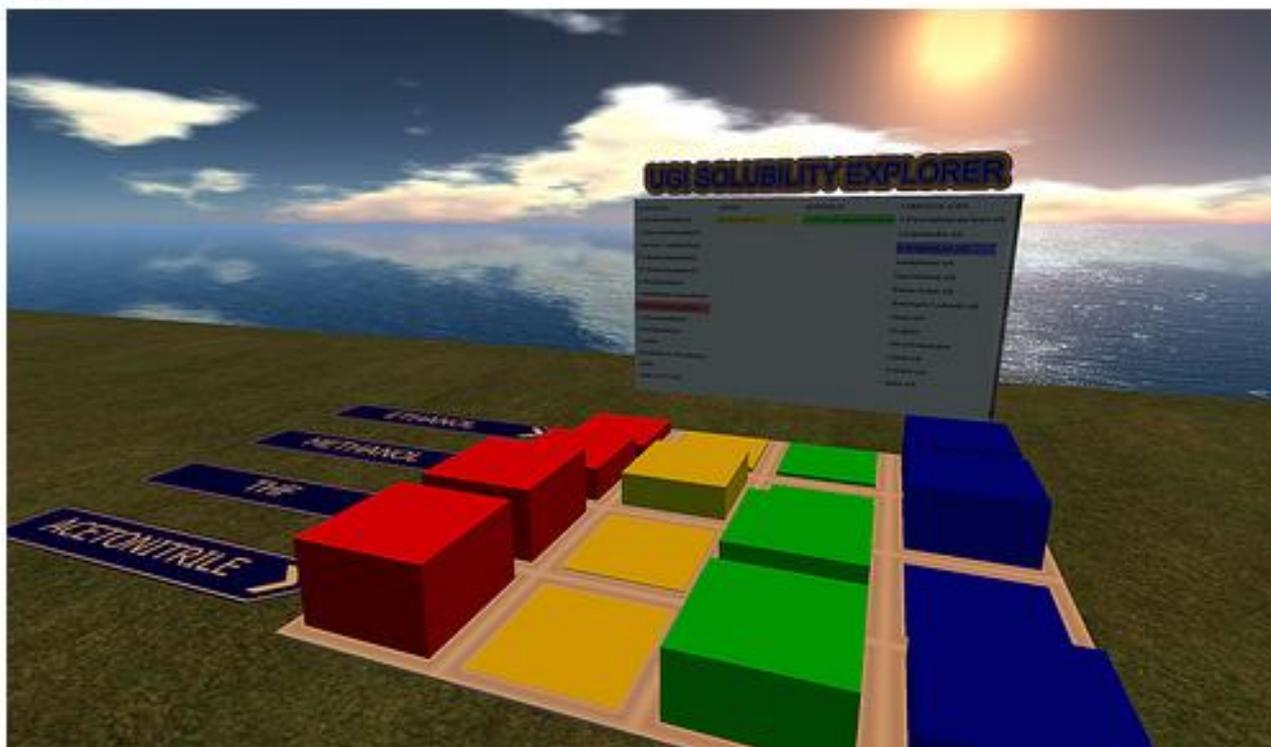


<http://oru.edu/ccda/sl/solubility/allsolvents.php?solute=4-nitrobenzaldehyde>

Exploring Solubility in Second Life (Andy Lang)

Ugi Solubility Data

ALL SIZES



Ugi solubility data from the open notebook science solubility challenge
(<http://onschallenge.wikispaces.com/>)
displayed in real-time in SL.

Visit it here: slurl.com/secondlife/ACS/231/114/25/

Pierre Lindenbaum's Solubility Data as RDF Triples

Validation Results

Your RDF document validated successfully.

Jump To:

[Source](#)

[Triples](#)

[Messages](#)

[Graph](#)

[Feedback](#)

[Back to](#)

[Validator Input](#)

Triples of the Data Model

Number	Subject	Predicate	Object
1	genid:A163010	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://us/Result
2	genid:A163010	http://usefulchem.blogspot.com/ontology/experiment-id	http://us
3	genid:A163010	http://usefulchem.blogspot.com/ontology/sample-id	sample:2
4	genid:A163010	http://usefulchem.blogspot.com/ontology/concentration	"1.32"^^c
5	compound:glycine_methyl_ester	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://us/Solute
6	genid:A163010	http://usefulchem.blogspot.com/ontology/solute	compound:

Results and Workflows in Machine-Friendly Format

☆ RESULT0001

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page ▾

[discussion](#)

[history](#)

[notify me](#)

SOURCE: <http://usefulchem.wikispaces.com/Exp150>

- ADD container (type=one dram screwcap vial)
- ADD compound (common name=methanol, InChIKey=OKKJLVBELUTLKV-UHFFFAOYAX, volume=1 ml)
- WAIT (time=15 min)
- ADD compound (common name=benzylamine, InChIKey=WGQKYBSKWIADBV-UHFFFAOYAL, volume=54.6 ul)
- VORTEX (time=15 s)
- WAIT (time=4 min)
- ADD compound (common name=phenanthrene-9-carboxaldehyde, InChIKey=QECIGCMPORCORE-UHFFFAOYAL, mass=103.1 mg)
- VORTEX (time=4 min)
- WAIT (time=22 min)
- ADD compound (common name=crotonic acid, InChIKey=LDHQCZJRKDOVOX-JSWHHWTPCJ, mass=43.0 mg)
- VORTEX (time=30 s)
- WAIT (time=14 min)
- ADD compound (common name=tert-butyl isocyanide, InChIKey=FAGLEPBREOX SAC-UHFFFAOYAL, volume=5 ul)
- VORTEX (time=5.5 min)
- TAKE PICTURE



Experiments in Chemical Markup Language

CMLUgiReaction - Google Docs - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://docs.google.com/Doc?id=dq5m5bs_12hb8d2wcv&hl=en_en_GB

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FriendFeed Google Reader (5) solubility of boc-Glycine in ... Jean-Claude says... Sortase Cloning Google Docs - All items CMLUgiReaction - Go...

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Verdana 10pt B U A Link

Menu Bar

[Link to Precedings Paper](#)
[Wiki page of paper03](#)

CMLReact for typical reaction: We have taken the page fEXP203 but we are not clear whether we have taken the right variant. Can you check that amounts, yields, etc are all consistent for one exemplar. The CML reads OK and JUMBO draws the reactants.

```
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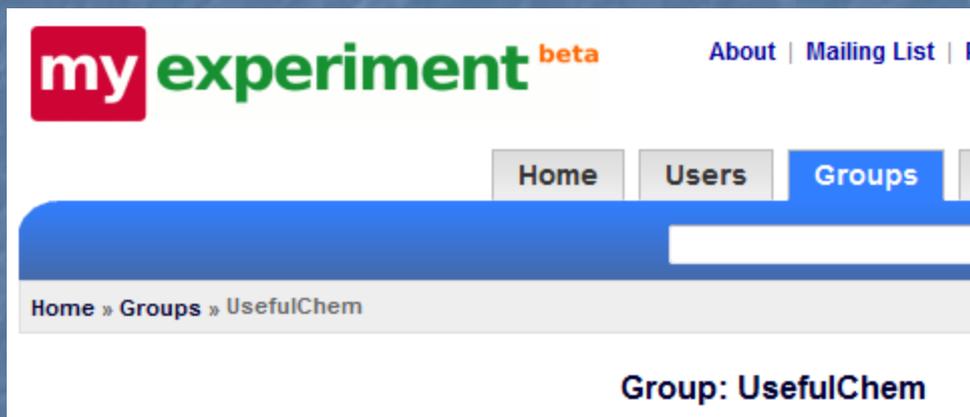
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Steps

1. Make up separate 1 mL of 1M solution
2. Take HMRs and CMRs of the aldehyde
3. Combine the two solutions into a 1 dr
4. Take HMR at 5, 10 and 20 minutes a
5. Take CMR at 25 min after mixing.
6. Take HMR at 40 min after mixing.
7. Take CMR at 45 min after mixing.
8. Take HMR at 80 mins after mixing.
9. Take CMR at 85 mins after mixing.

Workflow

Chemistry Plan

Monitoring the formation of an imine (v1)

View

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UsefulChem Project: Open Primary Research in Drug Design using Web2.0 tools

Rajarshi Guha
Indiana U

Tsu-Soo Tan
Nanyang Inst.

JC Bradley
Drexel U

Docking

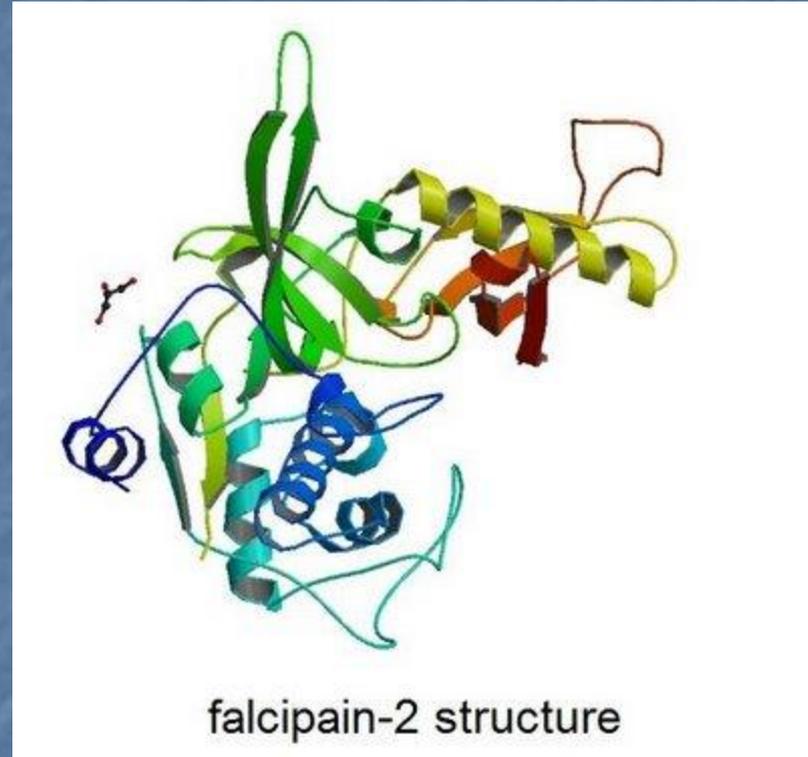
Synthesis

Phil Rosenthal
UCSF
(malaria)

Testing

Dan Zaharevitz
NCI
(tumors)

Malaria Target: falcipain-2 involved in hemoglobin metabolism



Architecture: Distributed, Interlinked and Redundant



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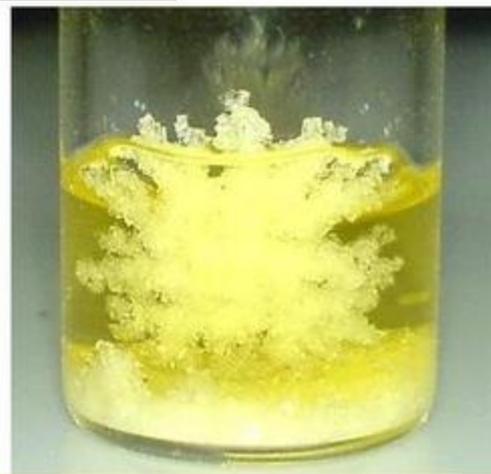
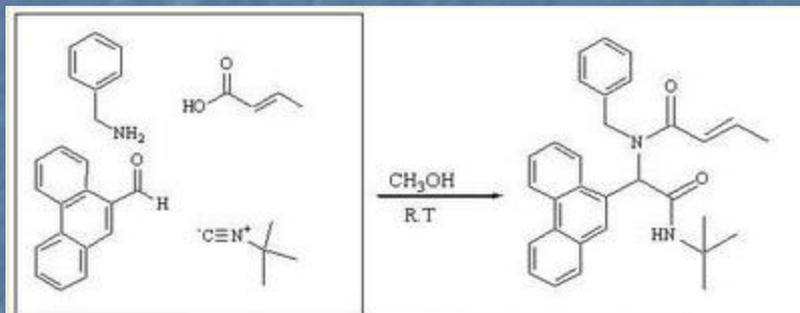
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TUESDAY, DECEMBER 11, 2007

➔ First Falcipain-2 Targets Shipped

We've reached an important milestone on our [CombiUgi](#) project involving the synthesis of falcipain-2 inhibitors. In my [last update](#) I described how our focus was more on doing many reactions in parallel and only looking for Ugi products that precipitate in pure form within a few days.

It took little longer than I hoped. [In order to do more reactions, we reduced our efforts towards monitoring.](#) One of the assumptions that we made was to trust a bottle's label to accurately describe its contents. That turned out to be [incorrect](#) for one of our key aldehydes, as we eventually found out by systematically taking NMRs of the starting materials. Soon after ordering a new bottle of phenanthrene-9-carboxaldehyde we were treated to the growth of beautiful crystals ([see EXP150](#) by Khalid and Emily):



Link to Lab Notebook Page in Wiki

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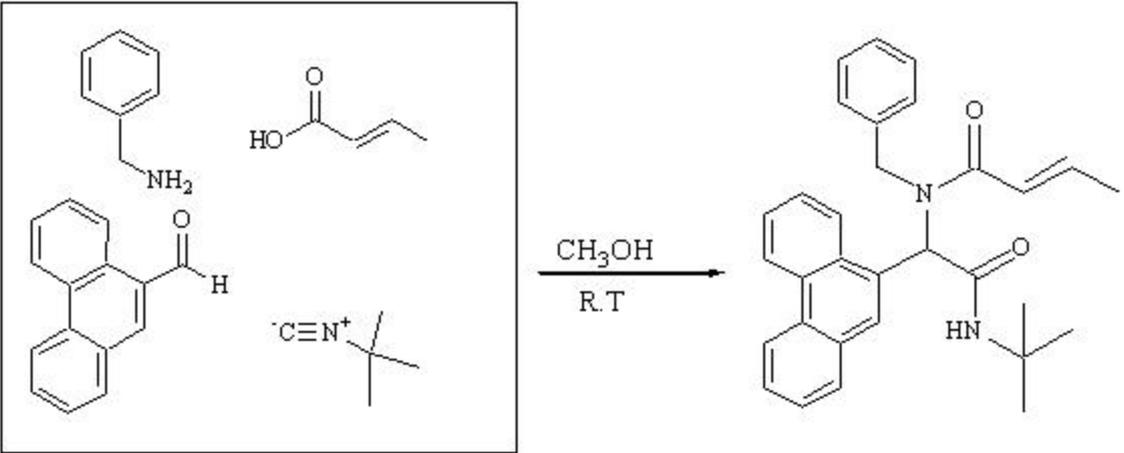
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- Libraries
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- Extra Credit
- Paper01 Draft
- Paper02 Draft
- Isolated Compounds
- Alicia's Masters Thesis
- CombiUgi Project
- Open Web Drug Dev.
- To Do List



Objective

To synthesize a [Ugi adduct](#)  from Phenanthrene-9-carboxaldehyde, benzylamine, *Tert*-butylisocyanide and Crotonic acid in methanol using Ugi 4CR following [Explan005](#). This is a repeat of [Exp143c](#). The target compound was ranked 155 in the [DEXP014-V1B](#)  file from [D-EXP014](#). The purpose of this experiment is to synthesize an anti-malarial compound based on the inhibition of falcipain-2, as described in this [summary post](#) .

[The experiment is repeated because the Phenanthrene-9-carboxaldehyde which was used in the previous experiment (Exp143) was acquired as a liquid. The aldehyde used here was obtained from Sigma Aldrich as a solid- Mpt-100C.]



<http://usefulchem.wikispaces.com/Exp150>

Link to Docking Procedure (Rajarshi Guha)

Objective

To dock CombiUgi [Library 3](#) (71K) against [falcipain-2](#) using Fred. All of the compounds in this library have starting materials in abundance in the Bradley lab. See [D-EXP012](#) for a similar docking run.

Procedure

The target of interest is the falcipain-2 enzyme. The crystal structure is available on the PDB ([1YVB](#)). This structure contains falcipain bound to cystatin and a glycerol along with some waters. The cystatin, glycerol and waters were removed for docking purposes. Since the complex is an example of a protein protein interaction, identifying the binding site was a bit tricky.

We identified two possible regions based on visual inspection as well as predicted hot-spot residues using the SPPIDER server (get the report [here](#)). This led to two sets of docking runs (V1 and V2). The important thing to note is that I don't know for sure whether these are the correct regions for a small molecule to interact and subsequently inhibit. V2 is probably a better bet, since it seemed reasonable visually and was also in the region of the residues predicted by SPPIDER.

Results

The rescored data files containing the final consensus scores and individual scores for each of the scoring schemes that was considered for the runs with the two binding sites named V1 and V2 (described in procedure)

[DEXP014-V1A](#) 56404 docked compounds in the V1 pocket of falcipain-2

[DEXP014-V1B](#) The first 1637 compounds of the above file. (Google Spreadsheet-shared file)

[DEXP014-V2A](#) 59402 docked compounds in the V2 pocket of falcipain-2

[DEXP014-V2B](#) The first 1500 compounds of the above file. (Google Spreadsheet-shared file)

Link to Docking Results: Lists of SMILES in GoogleDocs (Rajarshi Guha)

Google Docs BETA jeanclaud

D-EXP014-V1B-1to1637smiles Autosaved on Nov 1, 2007 3:00:57 PM EDT

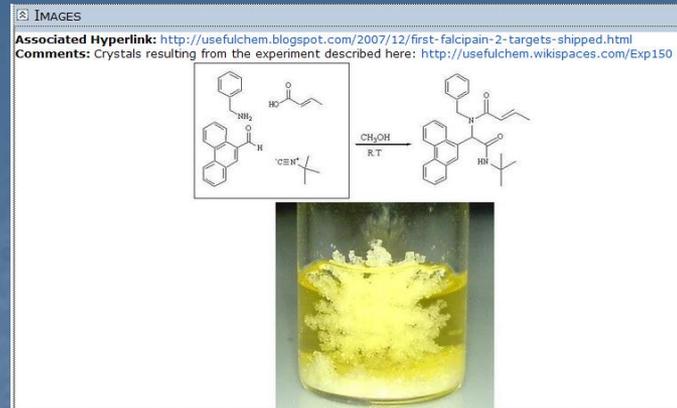
File Edit Sort Formulas Revisions

Undo Redo Cut Copy Paste Format Bold Italic Underline Text Color Background Color Table Border Text Color Merge across

	A	B
1	Smiles from D-Exp014V1A	Rank
2	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)CNC(=O)c4ccccc4</chem>	1
3	<chem>CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C)C(=O)CCc4ccc(cc4)OC</chem>	2
4	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)Cc4ccc(cc4)Cl</chem>	3
5	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)Cc4ccc(c(c4)O)O</chem>	4
6	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(Cc4ccccc4)C(=O)Cc5ccc(cc5)Cl</chem>	5
7	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(c4ccccc4)C(=O)Cc5ccc(cc5)Cl</chem>	6
8	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(c4ccccc4Cl)C(=O)Cc5ccc(cc5)Cl</chem>	7
9	<chem>CCCCCN(C(c1cc2ccccc2c3c1cccc3)C(=O)NCCCC)C(=O)C=CC</chem>	8
10	<chem>CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C4CCCC4)C(=O)Cc5ccc(cc5)Cl</chem>	9
11	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(Cc4ccccc4)C(=O)c5ccc5</chem>	10
12	<chem>CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C4CCCC4)C(=O)Cc5ccccc5</chem>	11
13	<chem>CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)Cc4ccc5c(c4)OCO5</chem>	12
14	<chem>Cc1ccc(cc1)S(=O)(=O)CNC(=O)C(c2ccccc2)N(Cc3ccc(o3)C)C(=O)c4ccccc4O)O</chem>	13
15	<chem>CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(Cc4ccccc4)C(=O)C(c5ccccc5)O</chem>	14
16	<chem>CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C4CCCC4)C(=O)Cc5ccc(c(c5)O)O</chem>	15

Comparing Experiments

Ugi Master Table



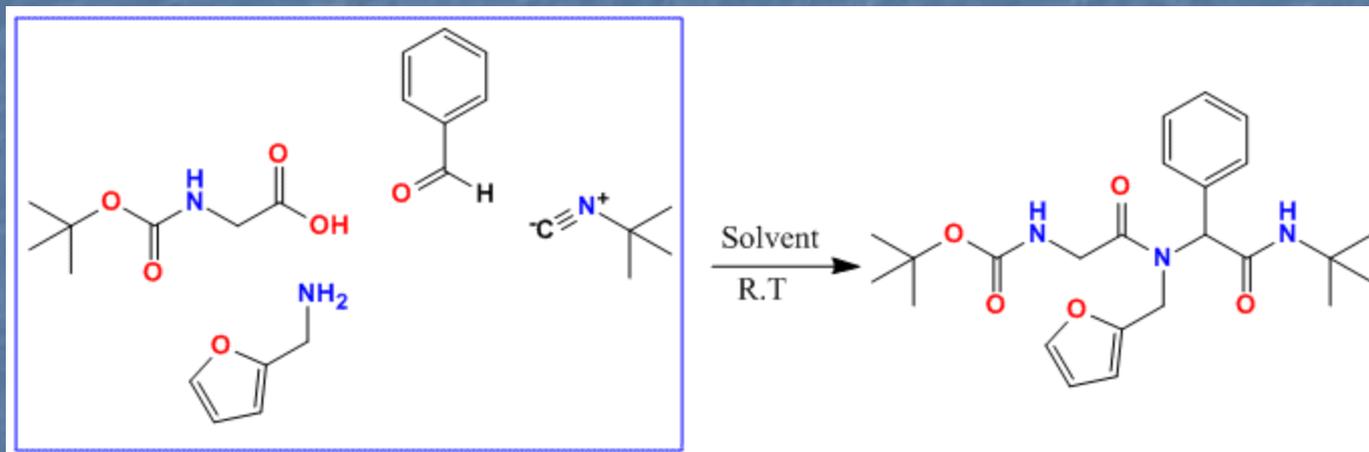
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jeanclaude.bradley@

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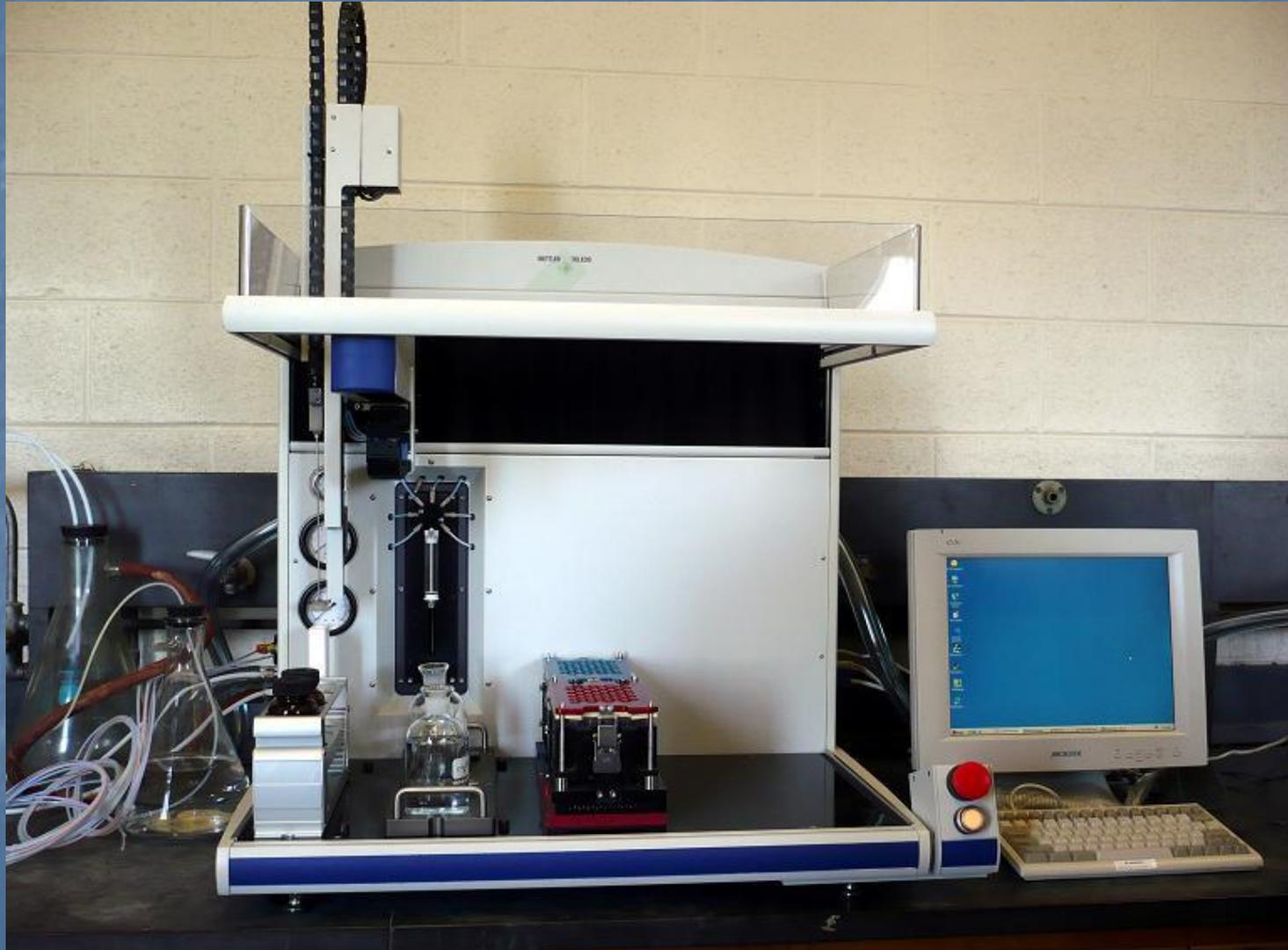
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3	socyanide	[C-]#[N+]C	Yes	50.1%	Khalid/Emily	methanol	1	0.5	0.5	0.5	0.5
4	socyanide	[C-]#[N+]C	Yes		Khalid	methanol	4	1.04	1.01	1	1
5	socyanide	[C-]#[N+]C	Yes		Khalid	methanol	4	2.09	2.66	1.99	1.97
6	socyanide	[C-]#[N+]C	Yes		Khalid	methanol	4	2	2.2	2	2
7	socyanide	[C-]#[N+]C	Yes	58.5%	Khalid/Emily	methanol	1	0.5	0.5	0.5	0.5
8	socyanide	[C-]#[N+]C	Yes		Khalid	methanol	4	2	2.2	2	2
9	socyanide	[C-]#[N+]C	Yes		Khalid	methanol	4	2	2.2	2	2
10	socyanide	[C-]#[N+]C	Yes		Alicia	methanol	4	1	1	1	1
11	socyanide	[C-]#[N+]C	Yes		Khalid	methanol	4	2	2.2	2	2
12	socyanide	[C-]#[N+]C	No		Rikesh	methanol	0.5	0.5	0.5	0.5	0.5
13	socyanide	[C-]#[N+]C	No		Rikesh	methanol	0.5	0.5	0.5	0.5	0.5
14	socyanide	[C-]#[N+]C	No		Rikesh	methanol	0.5	0.5	0.5	0.5	0.5
15	socyanide	[C-]#[N+]C	No		Rikesh	methanol	0.5	0.5	0.5	0.5	0.5
16	socyanide	[C-]#[N+]C	No		Rikesh	methanol	0.5	0.5	0.5	0.5	0.5
17	socyanide	[C-]#[N+]C	No		Rikesh	methanol	0.5	0.5	0.5	0.5	0.5

Reaction to Optimize



- Concentration (0.4, 0.2, 0.07 M)
- Solvent (methanol, ethanol, acetonitrile, THF)
- Excess of some reagents (1.2 eq.)

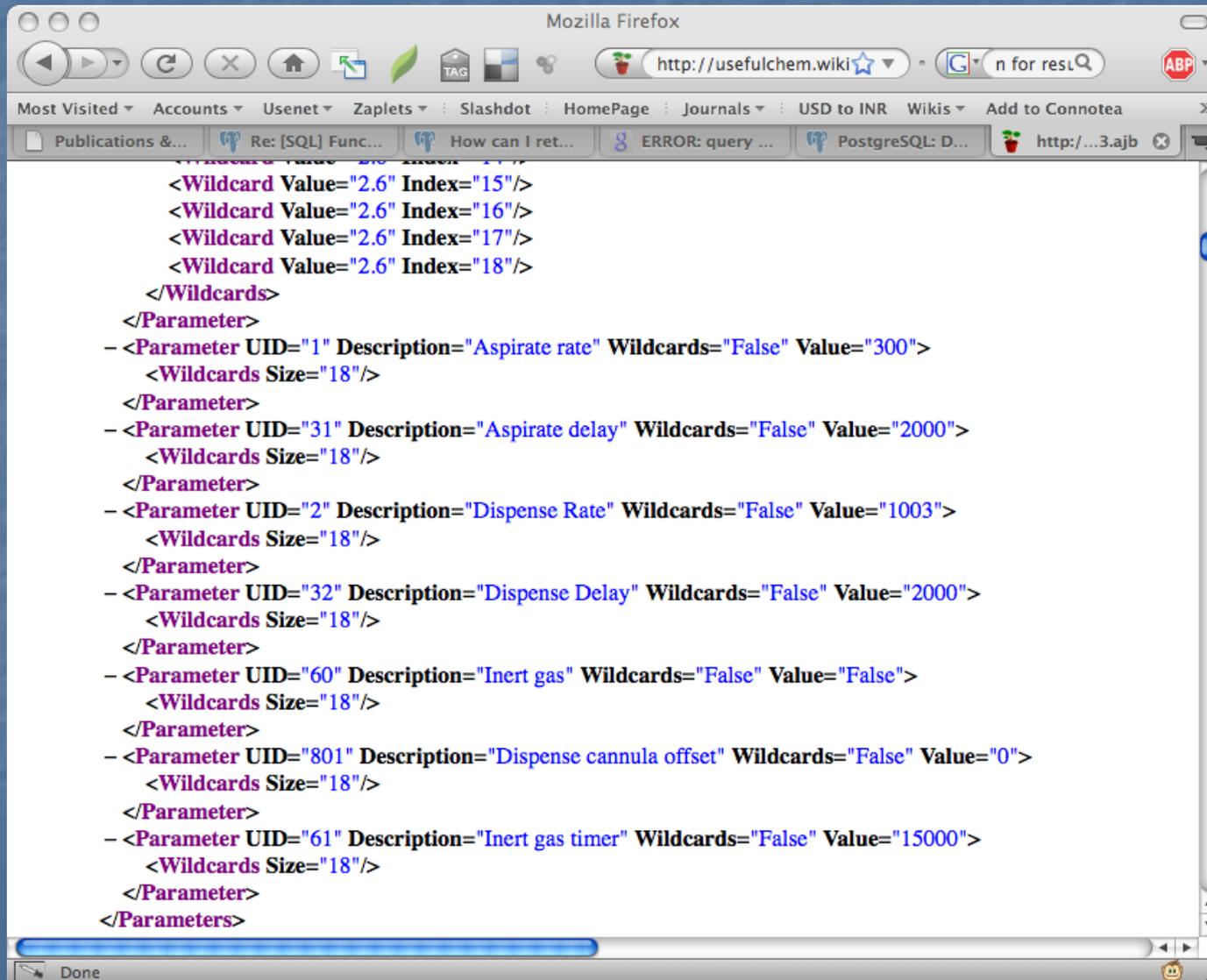
Mettler-Toledo MiniMapper



Mettler-Toledo MiniBlock System



XML reports from MiniMapper robot



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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	Run	Mini Block Rxn tube #	addition solvent	solvent amount (ml)	Ratios	Furfuryl (mL)	Benzaldehyde (mL)	Boc-gly (mL)	t-Butylamine (mL)	Furfuryl (mmol)	Benzaldehyde (mmol)	Boc-Gly (mmol)	t-Buiso (mmol)	Limiting Reagen (mmol)	Initial Wts of the reactor tubes (g)	Final Wts of the reactor tubes (g)	Wt of the Product (mg)	Yield Percent	average of groups of 6
2	1	A:2	methane	0.1	Eqimola Amine xs	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2	1.8858	1.9309	45.10	50.84	56.8912
3	2	A:4	methane	0.1	Ald xs	0.12	0.1	0.1	0.1	0.24	0.2	0.2	0.2	0.2	1.8796	1.9285	48.90	55.13	
4	3	A:6	methane	0.1	Acid xs tBUIC	0.1	0.12	0.1	0.1	0.2	0.24	0.2	0.2	0.2	1.8997	1.9505	50.80	57.27	
5	4	A:8	methane	0.1	Imine xs	0.1	0.1	0.12	0.1	0.2	0.2	0.24	0.2	0.2	1.844	1.884	40.00	45.09	
6	5	A:10	methane	0.1	Eqimola Amine xs	0.1	0.1	0.1	0.12	0.2	0.2	0.2	0.24	0.2	1.8819	1.9376	55.70	62.79	
7	6	A:12	methane	0.1	Ald xs	0.12	0.12	0.1	0.1	0.24	0.24	0.2	0.2	0.2	1.8548	1.9171	62.30	70.23	
8	7	B:1	methane	0.6	Eqimola Amine xs	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2	1.896	1.9198	23.80	26.83	51.3299
9	8	B:3	methane	0.6	Ald xs	0.12	0.1	0.1	0.1	0.24	0.2	0.2	0.2	0.2	1.8565	1.9021	45.60	51.41	
10	9	B:5	methane	0.6	Acid xs tBUIC	0.1	0.12	0.1	0.1	0.2	0.24	0.2	0.2	0.2	1.8992	1.9481	48.90	55.13	
11	10	B:7	methane	0.6		0.1	0.1	0.12	0.1	0.2	0.2	0.24	0.2	0.2	1.8766	1.9268	50.20	56.59	
12																			

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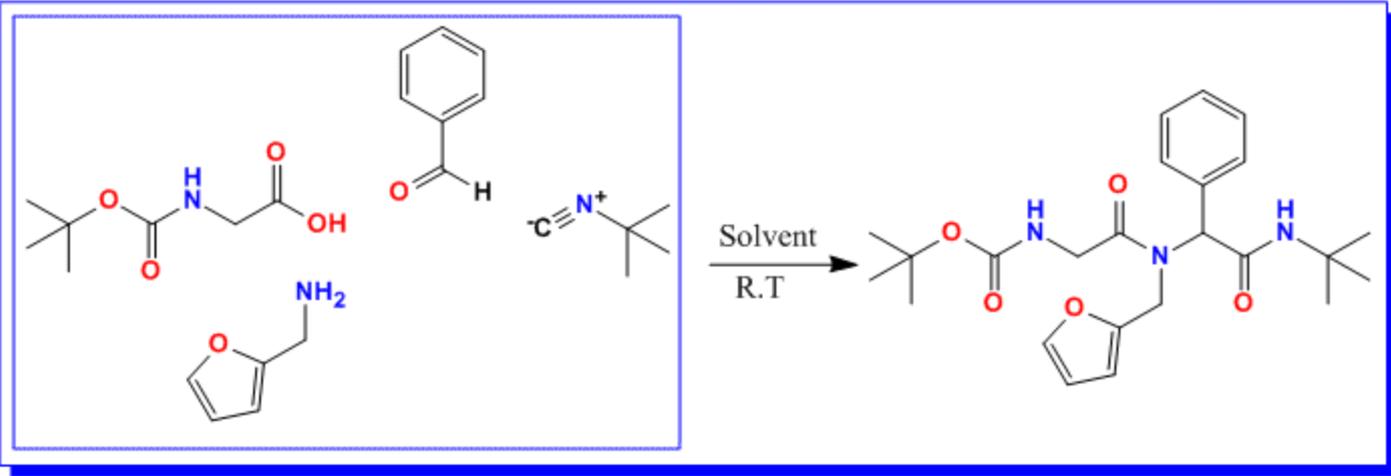
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Optimization of the Ugi reaction using parallel synthesis and automated liquid handling



Authors and Affiliations:
*Jean-Claude Bradley** Khalid Baig Mirza and Kevin Owens (Drexel University); Tom Osborne (Mettler-Toledo); Antony Williams (ChemSpider)

Introduction
The Ugi reaction has proved to be a convenient way to quickly create diverse libraries of compounds (1-3). It involves the reaction of an amine, an aldehyde, a carboxylic acid and an isonitrile typically in methanol at room temperature. The Ugi

References to papers, blog posts, lab notebook pages, raw data

References

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5. Sanudo, M.; Marcaccini, S.; Basurto, S.; Torroba, T. [Synthesis of 3-Hydroxy-6-oxo\[1,2,4\]triazin-1-yl Alaninamides, a New Class of Cyclic Dipeptidyl Ureas](#) J. Org. Chem. vol 71, p. 4578 (2006)
6. [MiniBlock catalog description](#)
7. [MiniMapper catalog description](#)
8. Bradley, J.-C. and Mirza, K. B. UsefulChem EXP201 <http://usefulchem.wikispaces.com/EXP201>
9. Bradley, J.-C. and Mirza, K. B. UsefulChem EXP202 <http://usefulchem.wikispaces.com/EXP202>
10. Bradley, J.-C. and Mirza, K. B. UsefulChem EXP203 <http://usefulchem.wikispaces.com/EXP203>
11. m.p. from compound UC-099C from EXP099 <http://usefulchem.wikispaces.com/EXP099>
12. H NMR spectrum 203A11 from UsefulChem EXP203 <http://usefulchem.wikispaces.com/EXP203>
13. C NMR spectrum 206A from UsefulChem EXP206 <http://usefulchem.wikispaces.com/EXP206>
14. IR spectrum from compound UC-099C from EXP099 <http://usefulchem.wikispaces.com/EXP099>
15. FAB-MS from compound UC-099C from EXP099 <http://usefulchem.wikispaces.com/EXP099>
16. Analysis details available at http://usefulchem.wikispaces.com/space/showimage/EXP201-203_KO-A.xls
17. Montgomery, D.C., [Design and Analysis of Experiments](#), 6th ed., Hoboken, NJ: John Wiley & Sons, Inc, 2005.
18. Tye, H. and Whittaker, M. [Use of a Design of Experiments approach for the optimisation of a microwave assisted Ugi reaction](#), Org. Biomol. Chem. vol 2, p. 813 (2004).

ChemSpider Automated Mark-up of Chemical Names

Experimental

The MiniMapper automated liquid handler was programmed to deliver liquids in the following sequence to empty filter tubes in **methanol**, **benzaldehyde** (2M in **methanol**), **boc-glycine** (2M in **methanol**) and **t-butyliisocyanide** (2M in **methanol**). The default in excess, 120 microliters were delivered. The MiniBlock was then **t-butyliisocyanide** for 16 hours before being filtered using each tube followed by 15 min shaking before filtering off. The tubes were then dried under **high vacuum in a dessicator** for at least 24 hours. The purity was assessed by ¹H NMR for one sample from each solvent system.

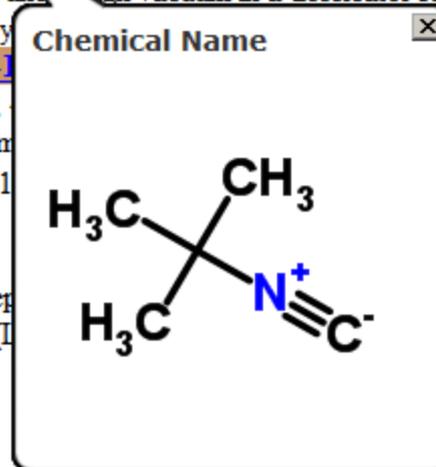
Characterization of the Ugi product **tert-butyl (2-[[2-(tert-butylamino)-2-oxo-1-phenylethylideneamino]ethyl]carbamate** (12, [spectrum](#)) (500MHz, δ ppm, **CDCl₃**) 1.33 (s, 9H), 1.45 (s, 9H), 4.21 (m, 2H), 7.19 (s, 1H), phenyl 7.21-7.37 (m, 5H); ¹³C NMR (13, [spectrum](#)) (500MHz, δ ppm) 155.7, 168.4 170.2; IR (14, [spectrum](#)) (*U*_{max} cm⁻¹ ATR): 1645,1673,1699, 3331

Data Analysis

The precipitate yield data was analyzed using the single-factor or two-factor (with regression) ANOVA analysis, Fisher's Least Significant Difference (LSD) test. The precipitate (17). All significance tests were performed at the 95% confidence level.

Results and Discussion

Figure 1 summarizes the effect of solvent composition on the yield of the Ugi precipitate. A single factor ANOVA indicates a



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Jean-Claude Bradley¹, Khalid Mirza¹, Kevin Owens¹, Tom Osborne², & Antony Williams³

Correspondence: [bradlejc\[at\]drexel.edu](mailto:bradlejc@drexel.edu)

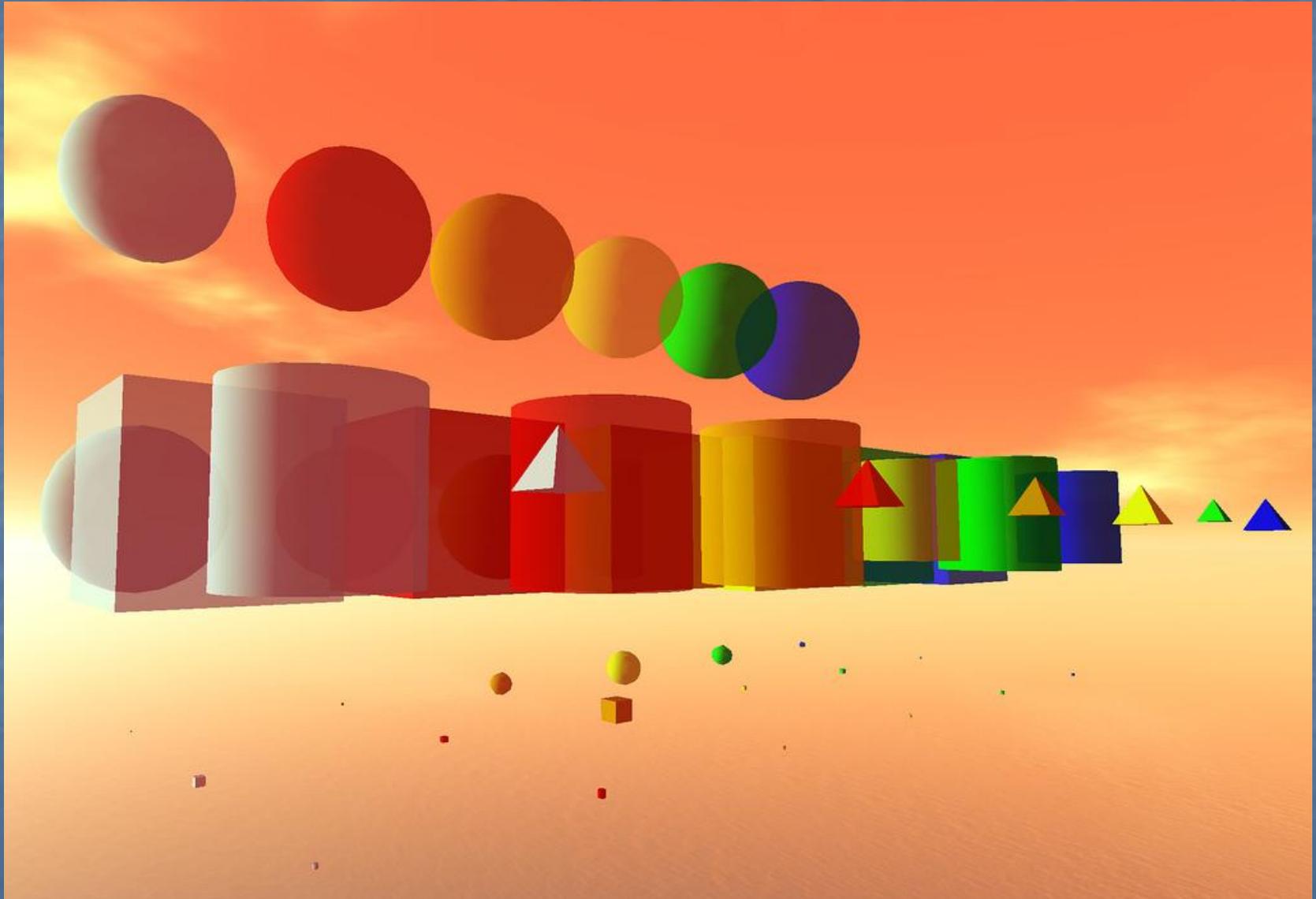
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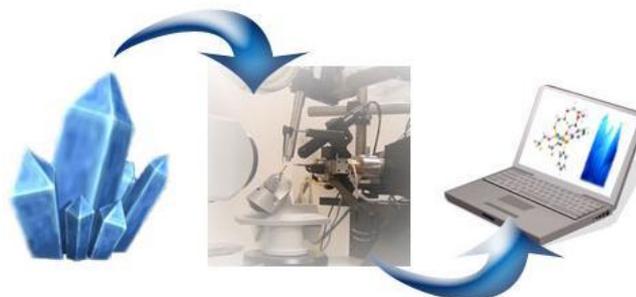
Reaction Optimization Visualization in Second Life





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UC150D

Drexel University^a
Youngstown^b

C31H32N2O2

InChI=1/C31H32N2O2/c1-5-13-28(34)33(21-22-14-7-6-8-15-22)29(30(35)
32-31(2,3)4)27-20-23-16-9-10-17-24(23)25-18-11-12-19-26(25)27/h5-
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Identification Number: 10.3737/ecrystals.chemistry.drexel.edu/1

Controlled Keywords: Ugi product

Date Created: 21 May 2008

Deposited On: 22 May 2008 17:05

Deposited: Jean-Claude Bradley

unspecified *

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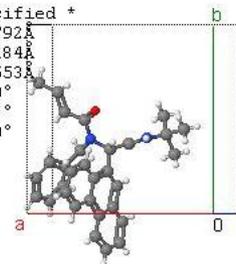
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$\alpha=90.0^\circ$

$\beta=95.2^\circ$

$\gamma=90.0^\circ$



Jmol

Available Files

Final Result

Collaborative Drug Discovery (CDD) Database

Collaborative Drug Discovery - Mozilla Firefox

View History Bookmarks Tools Help

https://www.collaborativedrug.com/queries

Google

Free Hotmail RealPlayer Windows Marketplace Collaborative Drug Di... Windows Media Collaborative Drug Di... Mozilla Firefox Start ... Mozilla Firefox Start ... Windows



COLLABORATIVE DRUG DISCOVERY
Drexel University

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Currently viewing my group's data only

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Mine Protocols and Molecules

Find Molecules by Protocol

(any protocol type)

(any protocol)

[Add a term](#)

Keywords

(any protocol)

Falcipain-2

Plasmodium Falciparum

Save this search as:

[Save](#)

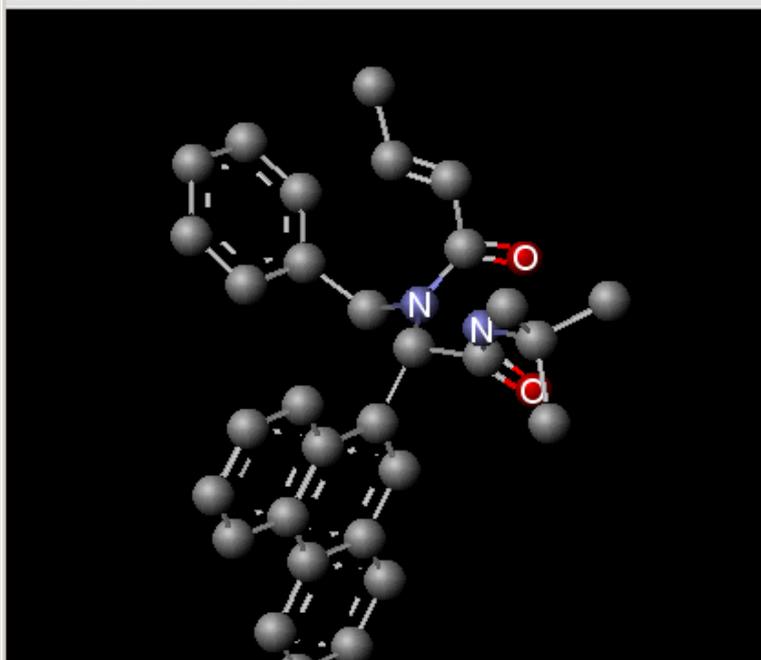
Search Results

[Export 1 result to Excel](#)

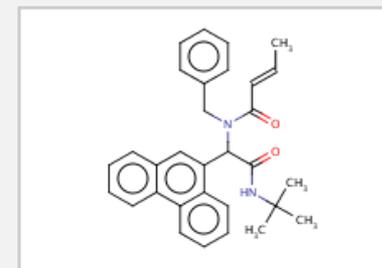
1 matching result

MarvinView

File Edit View Tools Help



Structure



Search by:

- substructure
 similarity

first 100 results

[Search Molecules](#)

Outcome of Guha-Bradley-Rosenthal collaboration

SAMPLE ID	Recombinant FP-2 Fluoroscan IC50 (nM)	Plasmodium falciparum strain W2 In Vitro IC 50 (nM) Flow	Enzyme target	Binding Site	Rank
148B	19655	7994	falcipain-2	V1	153
150D	16660	5411	falcipain-2	V1	155
175C	6621	1839	falcipain-2	V1	18
176C	8419	4853	falcipain-2	V1	29
171F/6-4	12752	~10000	falcipain-2	V2	6
171K/11-4	13170	>10000	falcipain-2	V2	11
173B/14	15330	~10000	falcipain-2	V2	14
173G19-4	50000	>10000	falcipain-2	V2	19
174K	12355	~10000	falcipain-2	V2	43
187-2A	>50000	>10000	none		
86B	50000	>10000	none		
62E	>50000	>10000	none		
104C	>50000	>10000	none		
64C	>50000	>10000	none		
99C	>50000	>10000	none		
108C	>50000	>10000	none		
109C	>50000	>10000	none		

Google Spreadsheet linked to Open Web Services = Chemistry Dashboard

	A	B	C	D	E	F
1	common name	mmol	density	MW	measure mg	measure microliters
2	benzaldehyde	1	1.045	106.122	106.1	102
3	ethanol	1.5	0.7893	46.0684	69.1	88
4	toluene	1.2	0.867	92.1384	110.6	128
5	formaldehyde	1	1.083	482.443	482.4	445
6	methanol	1	0.791	32.0419	32	41



Semi-Automated Measurement of solubility via web service analysis of JCAMP-DX files

Solute Lower Range (ppm)	Solute Upper Range (ppm)	Solute number of Hs	Solvent Lower Range (ppm)	Solvent Upper Range (ppm)	Solvent number of Hs	Concentration (M)
1.85	2	3	3.46	3.5	3	7.62
1.85	2	3	7.3	7.4	6	4.17

<http://usefulchem.blogspot.com/2009/03/semi-automated-measurement-of.html>

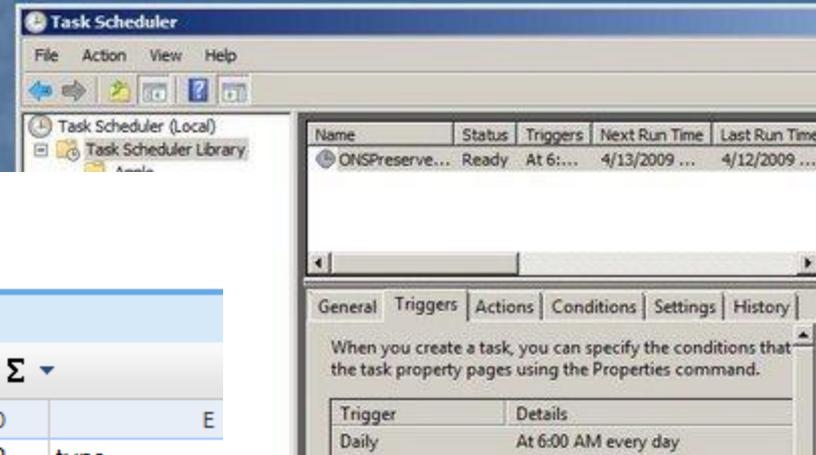
(Andy Lang)

Archiving and Curation of ONS and other new forms of scholarship?

Google Docs
BETA

ONSbackups

	A	B	C	D	E
	URL	name	wiki	EXP	type
2	http://spreadsheets.google.com/pub?key=plwwufp30hfq0udnEmRD1aQ&output=xls	SolSum	all	all	XLS
3	http://spreadsheets.google.com/pub?key=plwwufp30hfo3nECjaEuNMw&output=xls	ONSbackup	all	all	XLS
4	http://onschallenge.wikispaces.com/Exp075		ONSC	75	HTML
5	http://spreadsheets.google.com/pub?key=p8qCqj9hchQDnINJZzcDePw&output=xls	ONSCEXP074-2	ONSC	74	XLS
6	http://showme.physics.drexel.edu/mirza/Software/JCAMP/4-pyutanociacidTHF.dx		ONSC	74	JCAMP-DX
7	http://onschallenge.wikispaces.com/Exp074		ONSC	74	HTML
8	http://spreadsheets.google.com/pub?key=p4mrrUH5NPXLOpzMz-4rHfA&output=xls	ONSC-EXP073	ONSC	73	XLS



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File format:

What sheets?

What cells?
Example: C13, A1:D5, range name

Here's the URL:
<http://spreadsheets.google.com/pub?key=p8qCqj9hchQAGsA2ShpO7dw&output=xls>

<input type="checkbox"/>	Name	Date modified	Type	Size
	ONSBackups.csv	4/10/2009 10:16...	Microsoft Office ...	5 KB
	4_10_2009sprea...	4/10/2009 10:16...	Microsoft Office ...	80 KB
	4_10_2009sprea...	4/10/2009 10:16...	Microsoft Office ...	56 KB
	4_10_2009sprea...	4/10/2009 10:16...	Microsoft Office ...	78 KB
	4_10_2009sprea...	4/10/2009 10:16...	Microsoft Office ...	83 KB
	4_10_2009sprea...	4/10/2009 10:16...	Microsoft Office ...	453 KB
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	4_10_2009onsc...	4/10/2009 10:17...	Firefox Document	27 KB
	4_10_2009onsc...	4/10/2009 10:16...	COM_JENNYHAL...	25 KB
	4_10_2009onsc...	4/10/2009 10:16...	COM_JENNYHAL...	22 KB

Other Open Notebooks

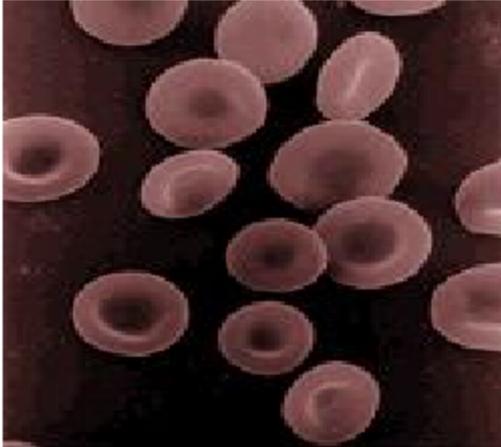
Gus Rosania's Notebook (recently terminated)

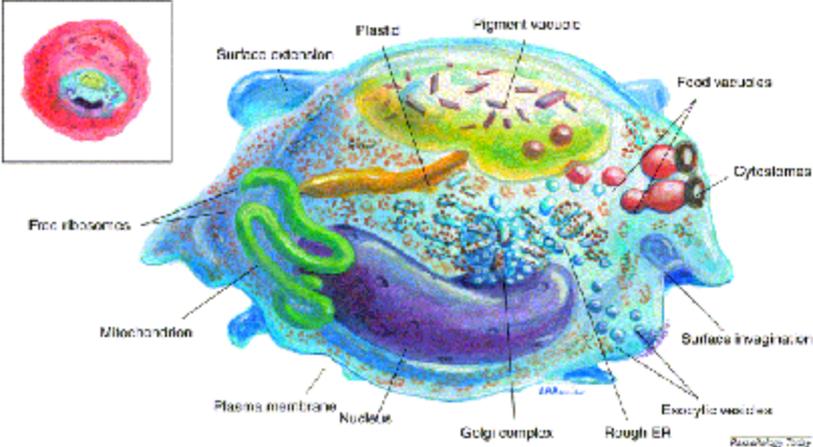
 **1CellPK** jcbradley · My Account

☆ RBC model in VCell [Edit This Page](#) page discussion history notify me

Virtual cell 4.4 beta version.

1. construct RBC plasmalemma,
2. construct separate model of RBC with parasite (parasite plasmalemma, food vacuole and mitochondrion) in trophozoite stage.





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- Jason Baik Project
- Xinyuan Project Blog
- Nan Project Blog
- Xinyuan's LabNotes
- Nan's LabNotes

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Cameron Neylon's Notebook

Sortase Cloning

Ligation of protein to oligonucleotides

21st October 2007 @ 14:24

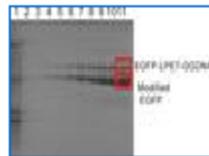
Post Type: protein_labelling

As will be discussed

<http://blog.openwetware.org/scienceintheopen/2007/11/18/an-experiment-in-open-notebook-science-sortase-mediated-protein-dna-ligation/>

I am putting up data that we have on a method for the attachment of oligonucleotides to DNA. This data is from experiments carried out by Lilyan Chan who is a student in my lab who is finishing up and therefore has not transferred to the open notebook.

Sortase was prepared by Lilyan Chan in our laboratory. GG-DNA **GG-PET2** was obtained from atdbio (www.atdbio.com). **EGFP-LPETGG-His6** was prepared in our lab. All reactions were carried out in **Sortase buffer**.



Experiment 1: Optimising target protein concentration

GG-DNA was ligated to EGFP-LPETGG-His6 protein using sortase A. Different concentrations of EGFP were used to find out optimal concentration to use in the future. Lane 1: Protein marker, lane 2: 0 μM EGFP, lane 3: 1 μM EGFP, lane 4: 5 μM EGFP, lane 5: 10 μM EGFP, lane 6: 20 μM EGFP, lane 7: 50 μM EGFP, lane 8: 75 μM EGFP, lane 9: 100 μM EGFP, lane 10: 150 μM EGFP, lane 11: 200 μM EGFP.

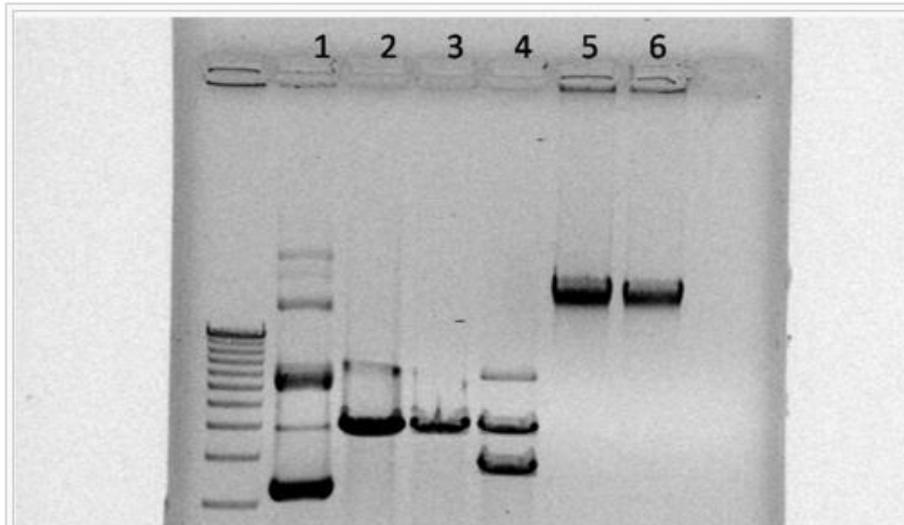
Anthony Salvagno's Notebook (Steve Koch group)

Results

I have an image of the gel results, but for some reason it didn't save right. Working on it.

According to the image of the gel, we got some pretty good data from cutting the plasmid with XhoI and NotI. It looks like there is an extra BstXI site in the plasmid which is why there are two bands (lane 4). We checked this on the map and sure enough there was an extra cutting site. Lane 1 provides the expected outcome (supercoiled DNA, nicked DNA, and regular DNA all in the same samples).

When the gDNA was cut with XhoI we didn't get as much a smear as we expected. You can see that the intensity of the fluorescence is not as bright in lane 6 as it is in lane 5 so we assume there was a little bit of cutting. The one solid band in lane 5 leads us to believe that we had some pretty clean DNA to begin with (no particulates, or sheared DNA).



SJK 14:22, 16 Feb

Acknowledgements

- Khalid Mirza (Drexel)
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- Antony Williams (ChemSpider)
- Andrew Lang (Oral Roberts U.)
- Rajarshi Guha (Indiana U.)
- Cameron Neylon (Southampton U.)