Open Notebook Science: Implications for the Future of Libraries

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April 2, 2008

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Traditional Lab Notebook (unpublished)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

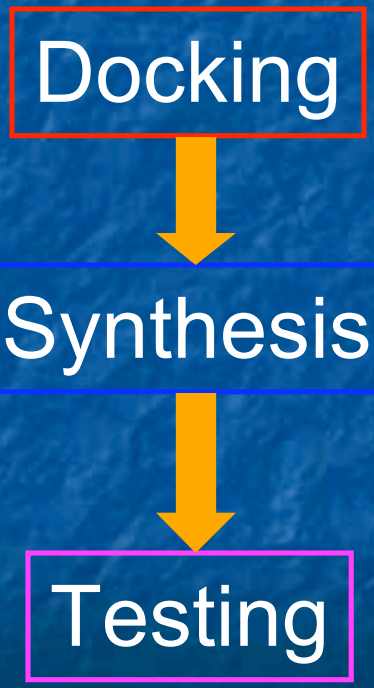
Archived Lectures Public and free online textbooks

Open Primary Research in Drug Design using Web2.0 tools (blogs, wikis, Second Life, mailing lists)

Rajarshi Guha
Indiana U

JC Bradley
Drexel U

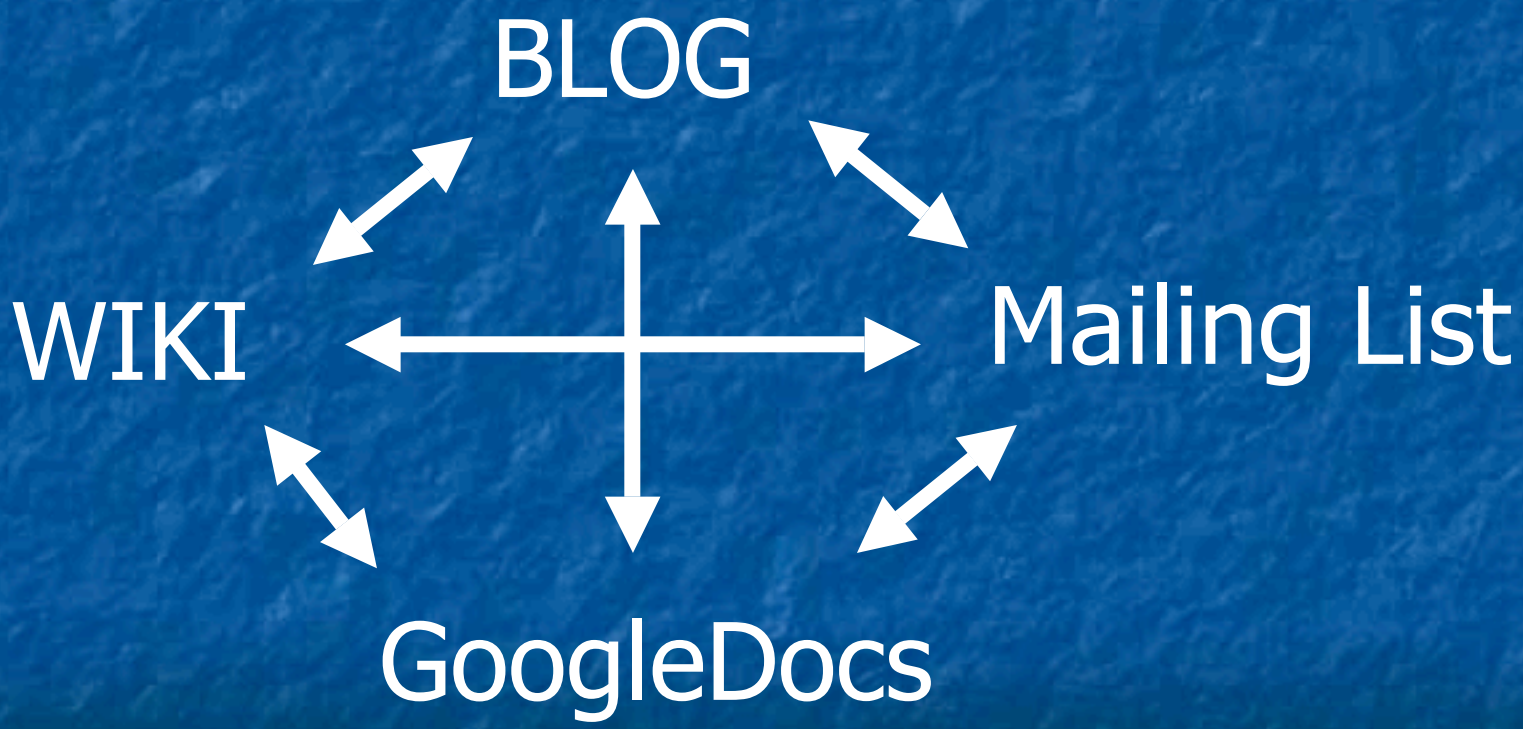
Phil Rosenthal
UCSF
(malaria)



Tsu-Soo Tan
Nanyang Inst.

Dan Zaharevitz
NCI
(tumors)

UsefulChem infrastructure



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Post specific partial solutions to these problems. Or execute a suggested ste
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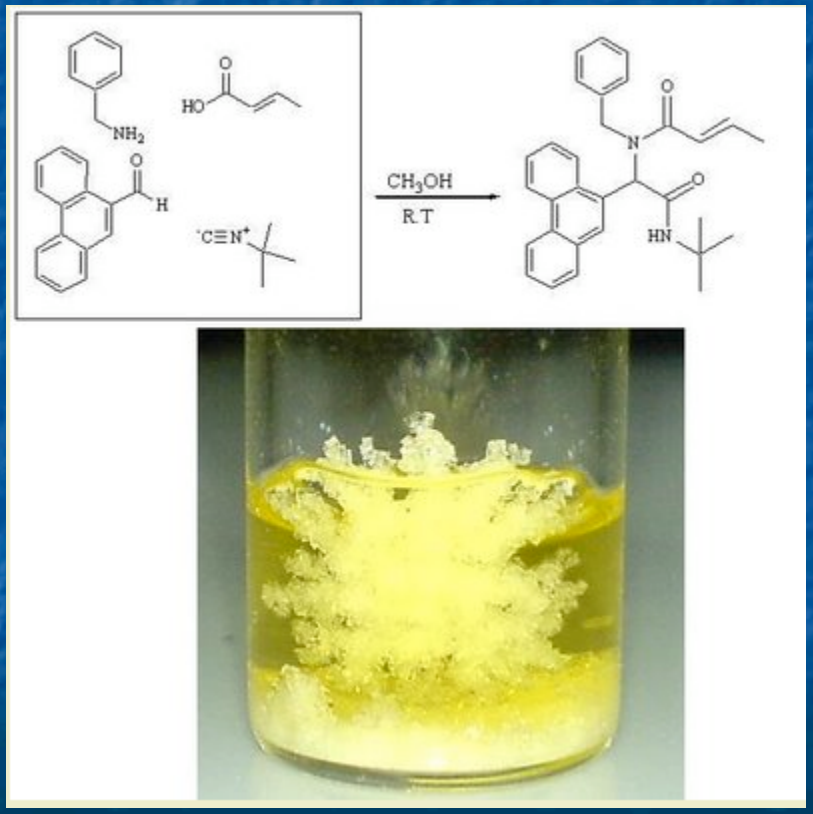
TUESDAY, DECEMBER 11, 2007

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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Exp150 | Edit This Page | page | discussion | history | notify me

Actions

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Navigation

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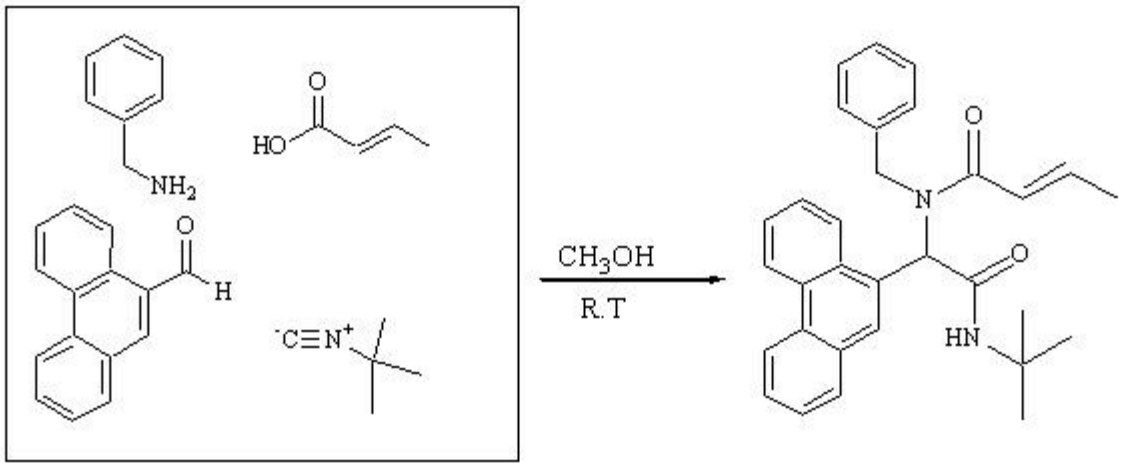
- Extra Credit
- Paper01 Draft
- Paper02 Draft
- Isolated Compounds
- Alicia's Masters Thesis
- CombiUgi Project
- Open Web Drug Dev.
- To Do List



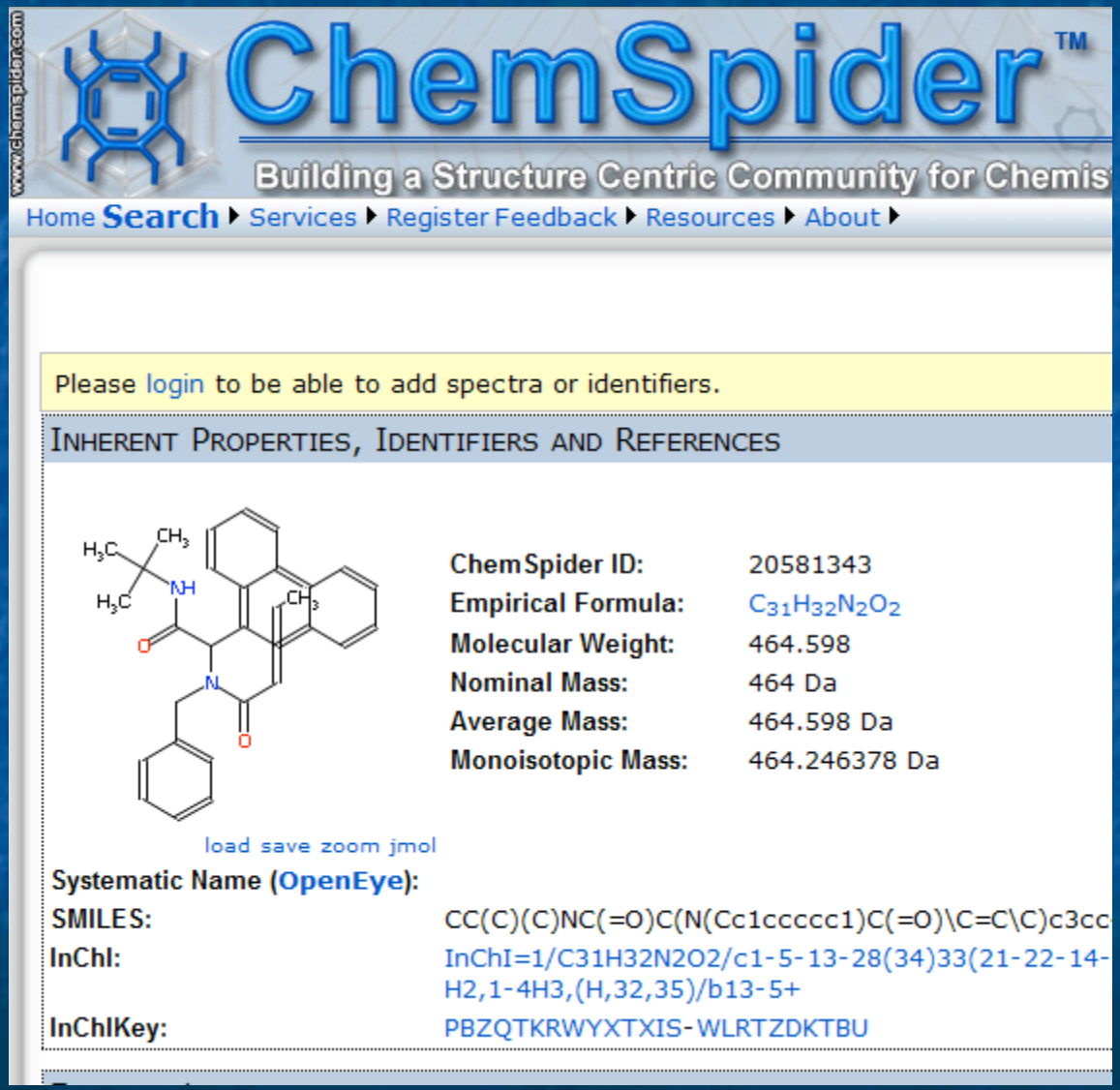
Objective

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 Molecules



Link to Experimental Plan

EXPLAN005 Edit This Page page discussion history notify me

Objective

To carry out Ugi reactions as quickly and as reproducibly as possible on small scales for products that precipitate out of methanol.

Steps

1. Weigh a 2 ml Eppendorf tube and write weight on the tube
2. Fill with 500 microliters of methanol
3. Add 500 micromoles of amine, aldehyde, acid and isonitrile in that order. After each addition, vortex for 15 seconds and confirm that a homogeneous solution has been obtained. If a clear solution is not obtained at any point abort.
4. Leave tube at room temperature for 24 hours.
5. Note the presence of a precipitate then vortex for 15 seconds.
6. Centrifuge at x RPM for 60 seconds then discard supernatant.
7. Add 500 microliters of methanol, vortex for 15 seconds then centrifuge at x RPM for 60 seconds.
8. Repeat the washing procedure for a total of 3 washes.
9. Put open tube under high vac for 15 minutes.
10. Record weight and obtain H and C NMR of entire sample in CDCl3.
11. Submit small sample for MS analysis.

Variations

1. Amine and Aldehyde can be mixed and left for 3 hours before addition of acid and isonitrile to see if it makes any difference.
2. One dram vials can be used instead of Eppendorf tubes.
3. Use vortexing or sonication to induce precipitation.

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 identfied 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 (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

Format | B | I | U | Abc | Align | Insert | Delete | Wrap Text | Merge across

	A	B
1	**Smiles from D-Exp014V1A**	**Rank**
2	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)CNC(=O)c4ccccc4	1
3	CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C)C(=O)CCc4ccc(cc4)OC	2
4	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)Cc4ccc(cc4)Cl	3
5	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)Cc4ccc(c(c4)O)O	4
6	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(Cc4ccco4)C(=O)Cc5ccc(cc5)Cl	5
7	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(c4ccccc4)C(=O)Cc5ccc(cc5)Cl	6
8	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(c4ccccc4Cl)C(=O)Cc5ccc(cc5)Cl	7
9	CCCCCCN(C(c1cc2ccccc2c3c1cccc3)C(=O)NCCCC)C(=O)C=CC	8
10	CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C4CCCCC4)C(=O)Cc5ccc(cc5)Cl	9
11	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(Cc4ccccc4)C(=O)c5ccco5	10
12	CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C4CCCCC4)C(=O)Cc5ccccc5	11
13	CCCCNC(=O)C(c1cc2ccccc2c3c1cccc3)N(CCC)C(=O)Cc4ccc5c(c4)OCO5	12
14	Cc1ccc(cc1)S(=O)(=O)CNC(=O)C(c2ccccc2)N(Cc3ccc(o3)C)C(=O)c4cccc(c4O)O	13
15	CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(Cc4ccco4)C(=O)C(c5ccccc5)O	14
16	CC(C)(C)NC(=O)C(c1cc2ccccc2c3c1cccc3)N(C4CCCCC4)C(=O)Cc5ccc(c(c5)O)O	15

Procedure Section

Procedure

To a one dram vial, charged with methanol (1 ml), benzylamine, phenanthrene-9-carboxaldehyde, crotonic acid and tert-butyl isonitrile (0.5mmol each) was added in that order. After each addition, the resulting solution was vortexed for 15 seconds (or more) and confirmed that a homogeneous solution had been obtained. The vial was capped tight and left at room temperature. After crystallization, the solution was decanted and the crystals were washed with methanol (3x 500uL) and dried under vacuum to obtain 150D in 58.5% yield.

Characterization of 150D: White powder; H-NMR (δ ppm ppm, CDCl3) 1.39 (s, 9H), 1.77 (d, 3H J 10.6Hz), 4.65-5.01 (m, 2H), 5.67 (s, 1H), 6.18 (d, 1H J 24.8 Hz), 6.33-6.81 (m, 4H), 6.88-7.23 (m 2H), 7.36-7.74 (m, 4H), 7.80 (d,1H J 12.2Hz), 7.90 (s 1H), 8.09 (d 1H J 12.2Hz), 8.51 (t 2H J 12.8Hz); 13C NMR (δ ppm, CDCl3) 18.1, 28.6, 49.0, 50.6, 51.7, 57.6, 94.6, 122.2, 122.4, 122.9, 124.2, 125.8, 126.6, 126.68, 127.1, 127.2, 128.7, 129.3, 130.1, 130.2, 130.4, 130.7, 130.9, 137.3, 143.4, 168.0, 269.9 ; IR (KBr, 1/cm): *v*=3323.75, 3058.46, 2969.65, 1677.58, 1655.43, 1594.01, 1526.84, 1421.50, 722.23, 695.58; HRMS *m/z* calcd for C31 H32 N2 O2 : 465.254202 [M+H] ***(compare same peak as found), list FAB results***, 487.236148 [M+Na]; found .

Link to Raw Data with JSpecView

Results

Phenanthrene-9-Carboxaldehyde (solid from S

HNMR

benzylamine

HNMR

Crotonic Acid

HNMR

***tert*-Butyl isocyanide**

HNMR

Characterization of 150D

add all good spectra to the ChemSpider entry

HNMR

CNMR

DEPT

MS (FAB) (link to raw data)

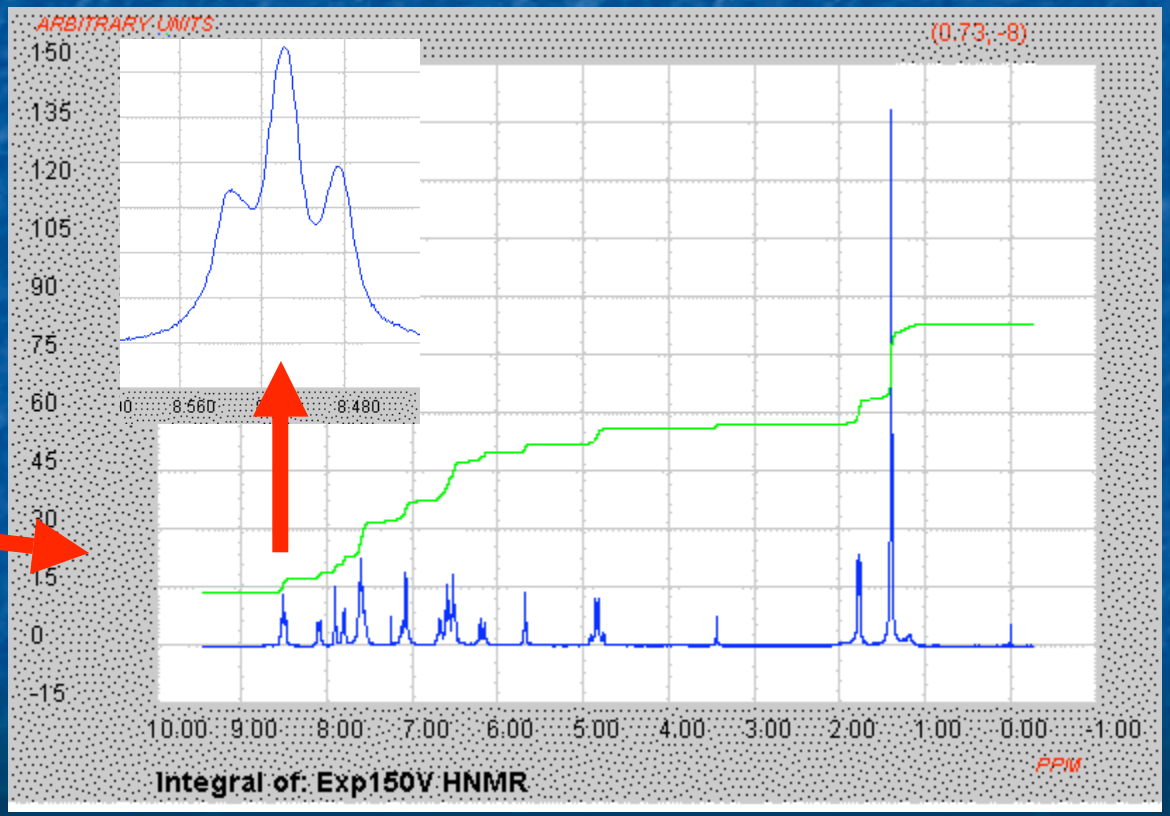
HRMS (link to raw data)

IR

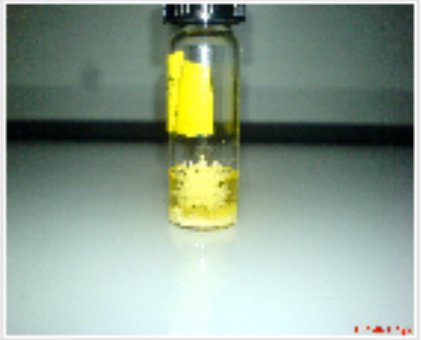
X- Ray studies

150D-Crystal Structure

150D-Crystal analysis



Conclusion is Fully Supported

6 min after mixing all components	15 h after mixing all components	17h After mixing all components
		

Discussion

All results are recorded in the Master Table of all Ugi synthesis attempts

Conclusion

The Ugi product was obtained in 59% yield.

Indexing the Experiments in Google

Tags

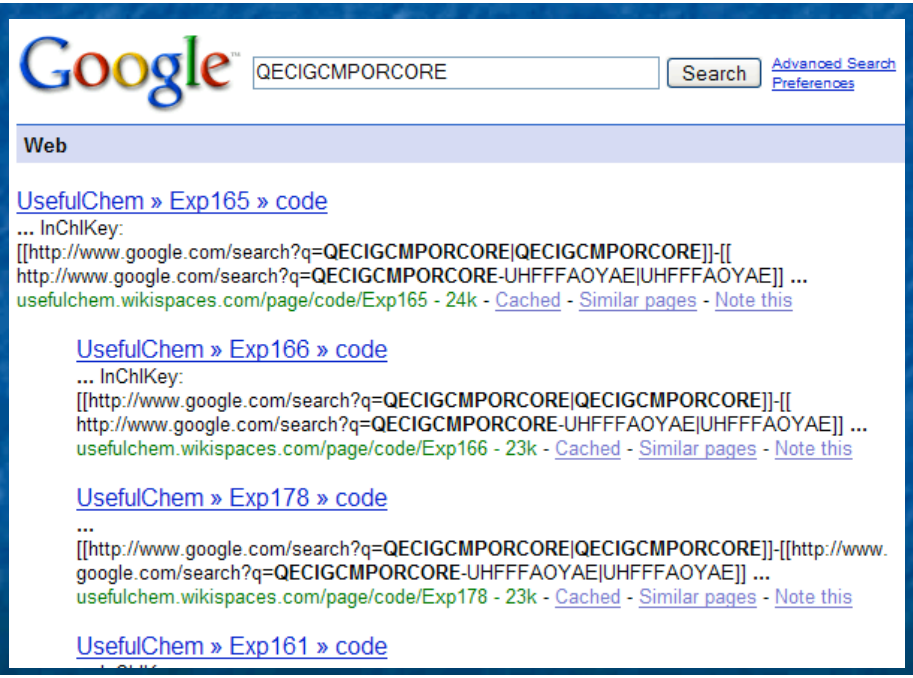
Phenanthrene-9-carboxaldehyde InChI=1/C15H10O/c16-10-12-9-11-5-1-2-6-13(11)15-8-4-3-7-14(12)15/h1-10H InChIKey: QECIGCMPORCORE-UHFFFAOYAE

tert-butylisocyanide InChI=1/C5H9N/c1-5(2,3)6-4/h1-3H3 InChIKey: FAGLEPBREOXSAC-UHFFFAOYAL

Crotonic Acid: InChI=1/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)/f/h5H InChIKey: LDHQCZJRKDOVOX-UHFFFAOYAC

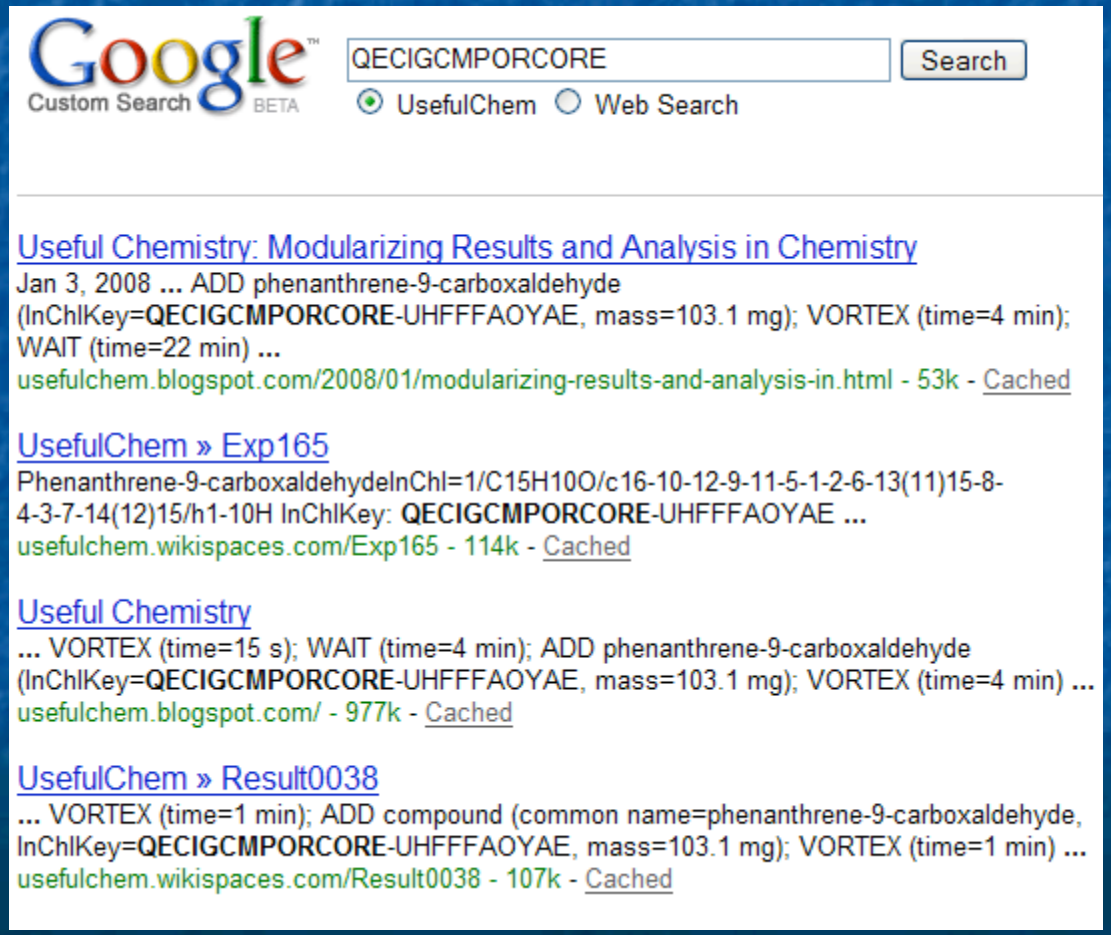
benzylamine InChI=1/C7H9N/c8-6-7-4-2-1-3-5-7/h1-5H,6,8H2 InChIKey: WGQKYBSKWIADBV-UHFFFAOYAL

Ugi Product



In order to show you the most relevant results, we have omitted some entries very similar to the 6 already displayed. If you like, you can repeat the search with the omitted results included.

Searching with Google Custom Search



How are people finding our experiments?

Specific Compounds

NMR in TFA
Phenylacetaldehyde
c4h6o2 nmr
methylene chloride/methanol
h'nmr of benzophenone
sulfuric acid pka
tertbutylamine
tosyl isocyanide
amino furan
dichloromethane polar?
Reaction between Benzaldehyde and NaBH4
phosphoric acid pka
veratraldehyde wiki

Experimental Conditions

kinetics boc deprotection
Rf value in polar solvent
why glycerol is immiscible with ether
side reaction of imines
5.8 ppm nmr
nmr cdcl3 chloroform side reaction
diasterotopic wiki
adding anhydrous MgSO4 to the dichlormethane ether extraction
hnmr doublet of doublet
Boc-protected NMR
chromatotron recipe
triplet cdcl3 "13c nmr"

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Big Picture

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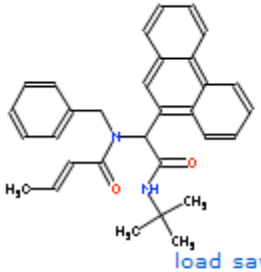
projects on QSAR & drug design
chemistry experiment results database

Using ChemSpider to archive compound characterization

Inherent Properties, Identifiers and References



load save zoom jmol

ChemSpider ID:	21105601
Empirical Formula:	$C_{31}H_{32}N_2O_2$
Molecular Weight:	464.598
Nominal Mass:	464 Da
Average Mass:	464.598 Da
Monoisotopic Mass:	464.246378 Da

> Support ChemSpider <

Systematic Name (OpenEye): (E)-N-benzyl-N-[2-(tert-butylamino)-2-oxo-1-(9-phenanthryl)ethyl]but-2-enamide

SMILES: CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O)\C=C\C)c3cc4ccccc4c2ccccc23

InChI: 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/h5-20,29H,21H2,1-4H3,(H,32,35)/b13-5+

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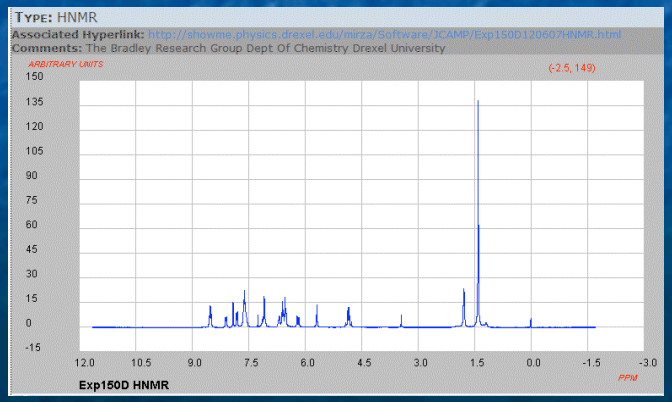
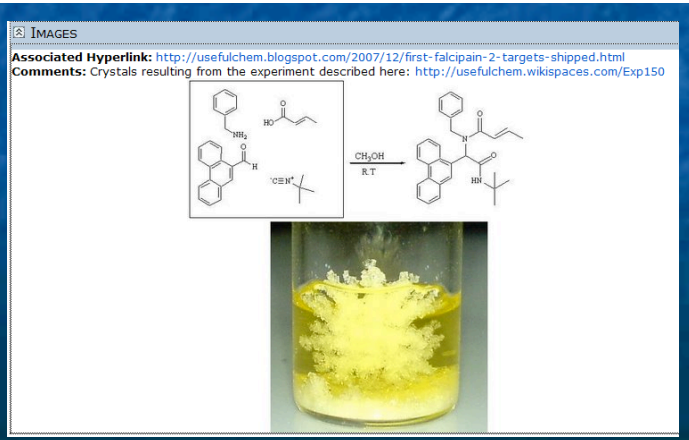
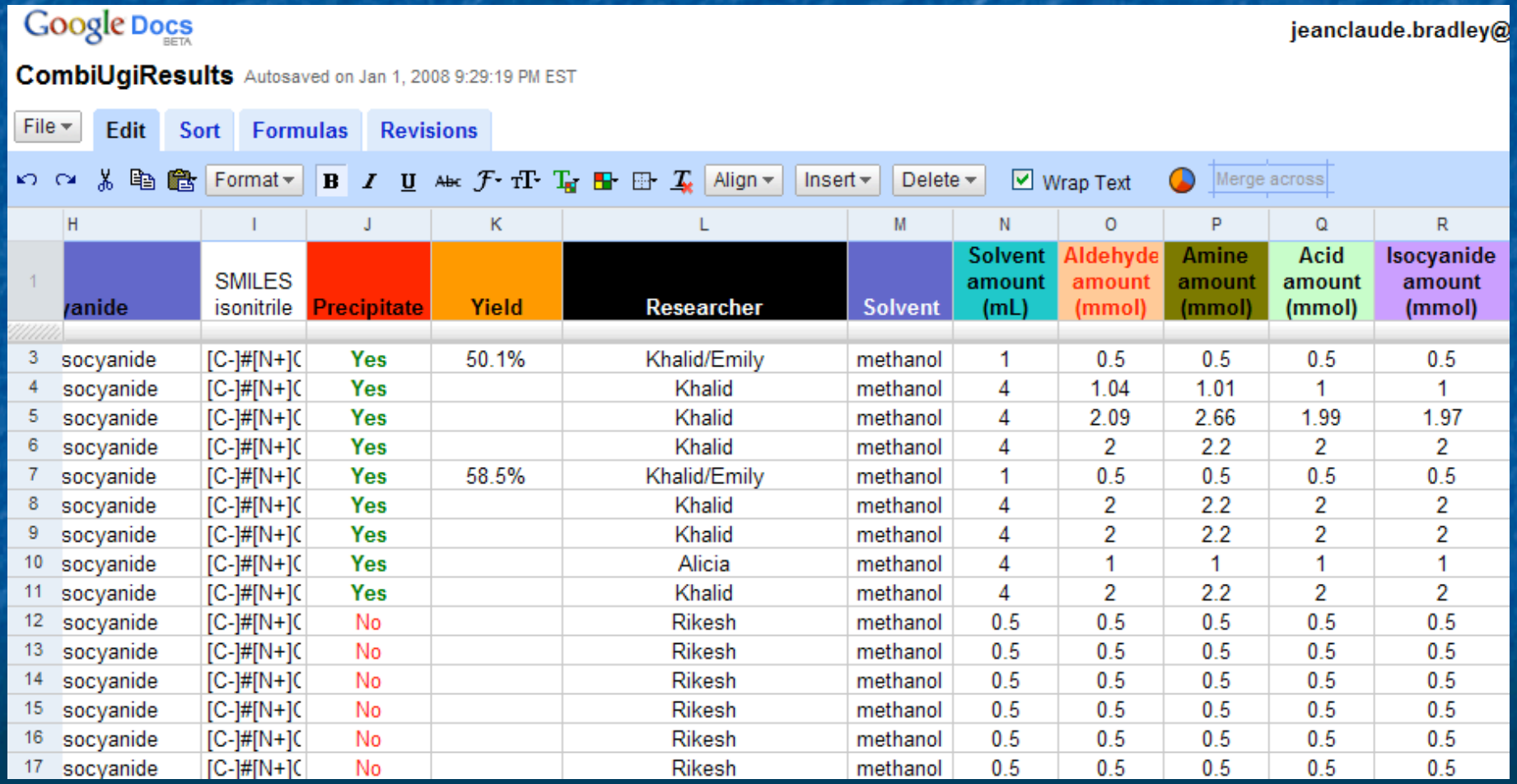




Comparing Experiments with GoogleDocs



Google Docs BETA

jeanclaude.bradley@

CombiUgiResults Autosaved on Jan 1, 2008 9:29:19 PM EST

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	H	I	J	K	L	M	N	O	P	Q	R
1	yanide	SMILES isonitrile	Precipitate	Yield	Researcher	Solvent	Solvent amount (mL)	Aldehyde amount (mmol)	Amine amount (mmol)	Acid amount (mmol)	Isocyanide amount (mmol)
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

The Most Important Section!

Log

2007-11-27

19:30- Charged a vial with 1ml of methanol and began to weigh out the crotonic acid and phenanthrene-9-carboxaldehyde.
19:40- Added 54.61 ul of benzylamine into the vial and vortexted for 15 seconds. A clear solution was achieved.
19:44- Added 103.1 mg of phenanthrene-9-carboxaldehyde to the vial and vortexed for one minute. The solution was light yellow and somewhat cloudy, and the sediment settled to the bottom of the vial. Therefore the solution was vortexed for another three minutes. The solid now went in to the solution, however a few oil like droplets were observed at the bottom of the vial. The solution homogenized upon standing.
20:10- Weighed out and added 43.0 mg of crotonic acid into the vial and vortexed for 30 seconds. The solution became clear.
20:25- Added 56.5 ul of tert-butyl isocyanide to the vial and vortexed for 30 seconds. The solution became cloudy with a few small flakes on the bottom of the vial. It was vortexed for a total of five more minutes before a clear yellow solution was obtained.
20:31 Obtained a picture of the vial (**150A**) ***remember to always label results so you can discuss them***
20:35- The vial was left to sit at room temperature for a day.

2007-11-28

11:23 Moved the vial to another location and obtained a picture of **150B**, still a clear solution..
12:18 Crystallization has started in.
13:29 Obtained another picture (**150C**)

Results in Machine-Friendly Format

RESULT0001 | Edit This Page | 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-UHFFFAOYA 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=FAGLEPBREOXSAC-UHFFFAOYAL, volume=
- VORTEX (time=5.5 min)
- TAKE PICTURE

Comparing Results in a Table

Google Docs BETA

jeanclaude.bradley@gma

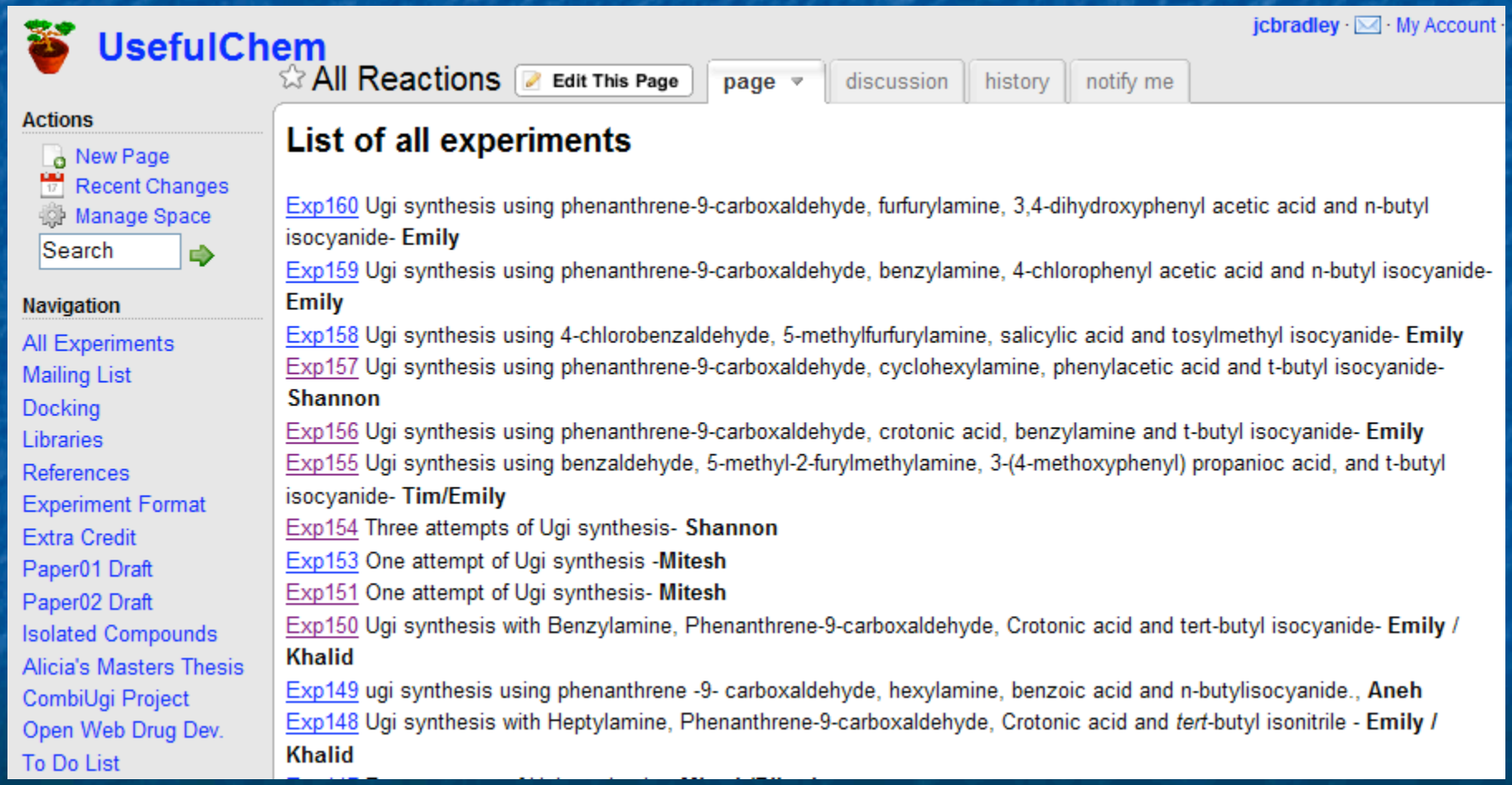
UgiWorkflows Autosaved on Jan 19, 2008 7:18:12 AM EST

File | Edit | Sort | Formulas | Revisions

Format | B | I | U | Abc | Align | Insert | Delete | Wrap Text | Merge across

	A	B	C	D	E	F	G	H	I	J
1	Workflow	result type	result	result ID	exp link	solvent	amine	vortex1	aldehyde	vortex2
2	1	picture	http://www.flickr	150A	http://usefulchem.wikispaces.com/Exp150	1	15	16	19	20
3	2	picture	http://www.flickr	150B	http://usefulchem.wikispaces.com/Exp150	1	15	16	19	20
4	3	picture	http://www.flickr	150C	http://usefulchem.wikispaces.com/Exp150	1	15	16	19	20
5	4	H NMR	http://showme.p	150D	http://usefulchem.wikispaces.com/Exp150	1	15	16	19	20
6	5	weight	138.5 mg	150D	http://usefulchem.wikispaces.com/Exp150	1	15	16	19	20
7	6	C NMR	http://showme.p	150D	http://usefulchem.wikispaces.com/Exp150	1	15	16	19	20
8	7	IR	http://showme.p	150D	http://usefulchem.wikispaces.com/Exp150	1	15	16	19	20

Table of Contents



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- Isolated Compounds
- Alicia's Masters Thesis
- CombiUgi Project
- Open Web Drug Dev.
- To Do List

List of all experiments

Exp160 Ugi synthesis using phenanthrene-9-carboxaldehyde, furfurylamine, 3,4-dihydroxyphenyl acetic acid and n-butyl isocyanide- **Emily**

Exp159 Ugi synthesis using phenanthrene-9-carboxaldehyde, benzylamine, 4-chlorophenyl acetic acid and n-butyl isocyanide- **Emily**

Exp158 Ugi synthesis using 4-chlorobenzaldehyde, 5-methylfurfurylamine, salicylic acid and tosylmethyl isocyanide- **Emily**

Exp157 Ugi synthesis using phenanthrene-9-carboxaldehyde, cyclohexylamine, phenylacetic acid and t-butyl isocyanide- **Shannon**

Exp156 Ugi synthesis using phenanthrene-9-carboxaldehyde, crotonic acid, benzylamine and t-butyl isocyanide- **Emily**

Exp155 Ugi synthesis using benzaldehyde, 5-methyl-2-furylmethylamine, 3-(4-methoxyphenyl) propanioc acid, and t-butyl isocyanide- **Tim/Emily**

Exp154 Three attempts of Ugi synthesis- **Shannon**

Exp153 One attempt of Ugi synthesis -**Mitesh**

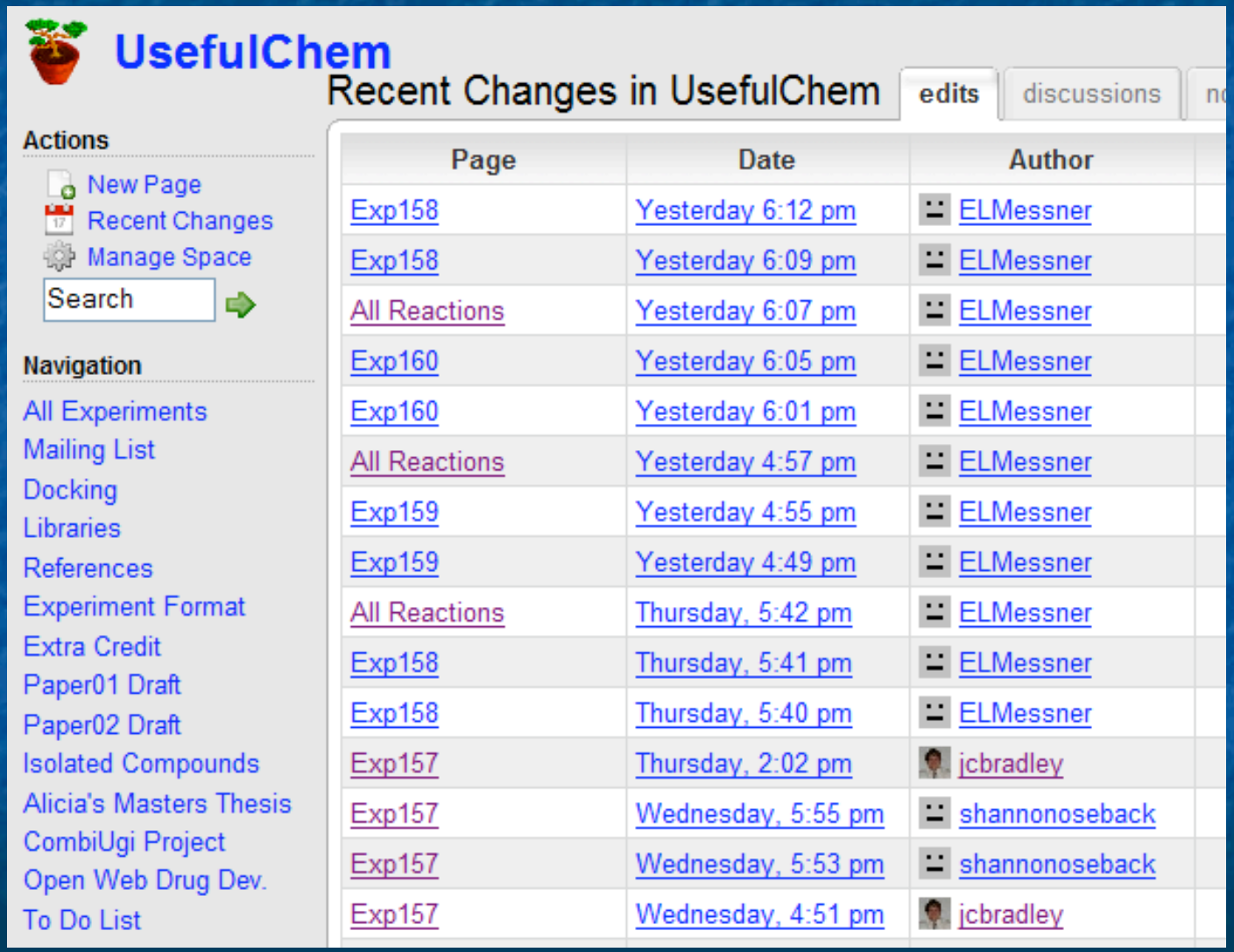
Exp151 One attempt of Ugi synthesis- **Mitesh**

Exp150 Ugi synthesis with Benzylamine, Phenanthrene-9-carboxaldehyde, Crotonic acid and tert-butyl isocyanide- **Emily / Khalid**

Exp149 ugi synthesis using phenanthrene -9- carboxaldehyde, hexylamine, benzoic acid and n-butylisocyanide., **Aneh**

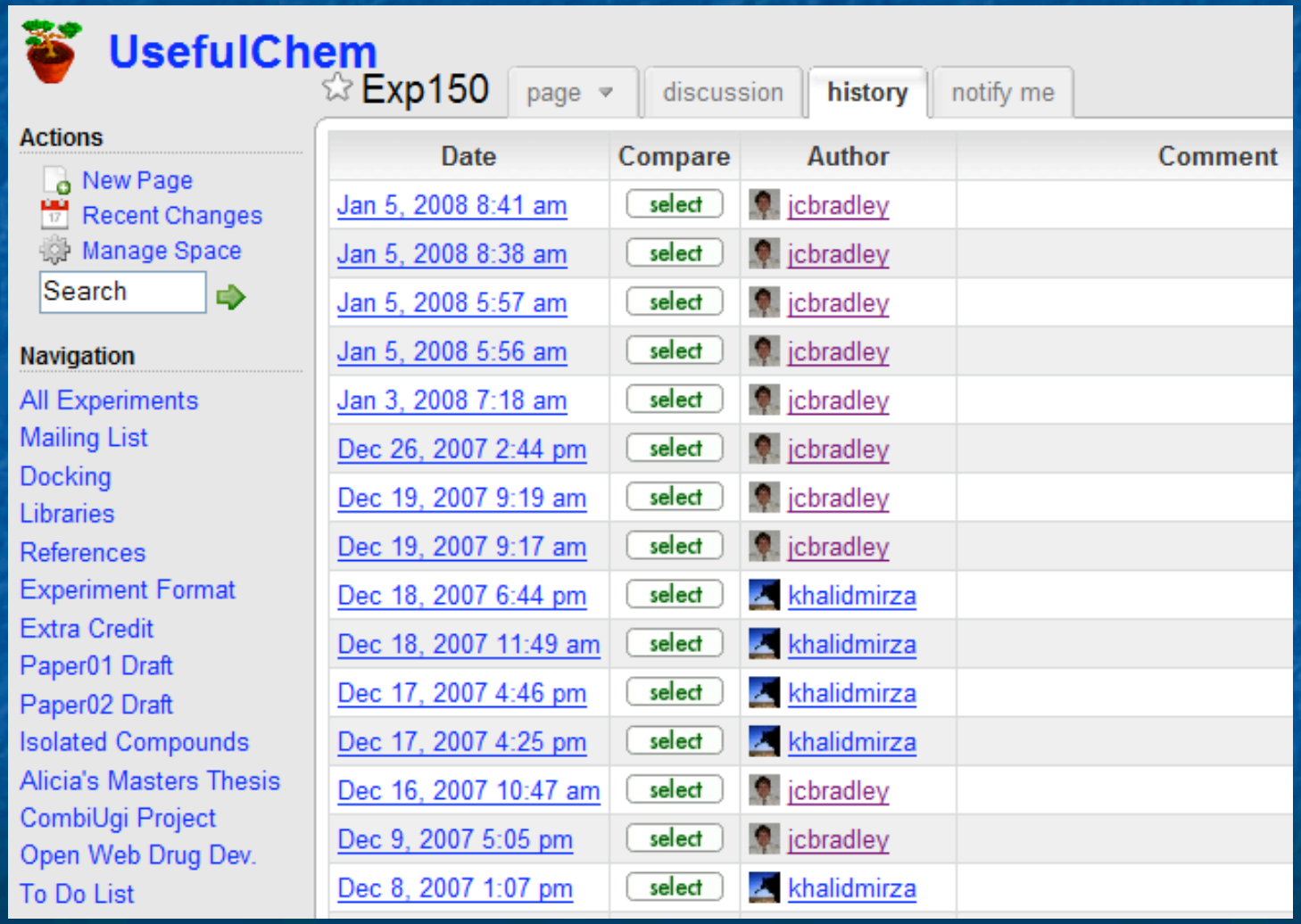
Exp148 Ugi synthesis with Heptylamine, Phenanthrene-9-carboxaldehyde, Crotonic acid and *tert*-butyl isonitrile - **Emily / Khalid**

Recent Changes in Wiki



Page	Date	Author
Exp158	Yesterday 6:12 pm	ELMessner
Exp158	Yesterday 6:09 pm	ELMessner
All Reactions	Yesterday 6:07 pm	ELMessner
Exp160	Yesterday 6:05 pm	ELMessner
Exp160	Yesterday 6:01 pm	ELMessner
All Reactions	Yesterday 4:57 pm	ELMessner
Exp159	Yesterday 4:55 pm	ELMessner
Exp159	Yesterday 4:49 pm	ELMessner
All Reactions	Thursday, 5:42 pm	ELMessner
Exp158	Thursday, 5:41 pm	ELMessner
Exp158	Thursday, 5:40 pm	ELMessner
Exp157	Thursday, 2:02 pm	jcbradley
Exp157	Wednesday, 5:55 pm	shannonoseback
Exp157	Wednesday, 5:53 pm	shannonoseback
Exp157	Wednesday, 4:51 pm	jcbradley

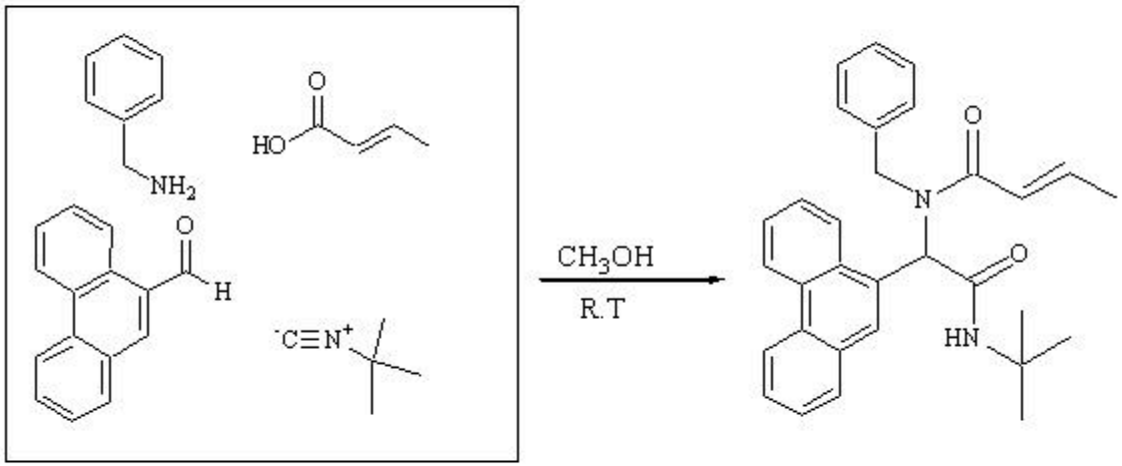
Tracking Versions of Wiki Pages



Comparing Versions of Wiki Pages

Exp150 | page | discussion | **history** | notify me

Dates: Dec 18, 2007 6:44 pm to Jan 5, 2008 8:41 am
Actions: show wikitext changes
Key: Inserted Text Deleted Text Jump To: First Last



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 Exp143 c.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 .

Telling the story of the failures

Synthesis of DOPAL

DOPAL is a key intermediate in the Ugi synthesis of many of the diketopiperazine anti-malarial targets we are synthesizing. Since we have not found a commercial source, we have been trying to make it by treating adrenaline with acid, based on a convenient but low yielding one-step decomposition of adrenaline in 85% phosphoric acid.

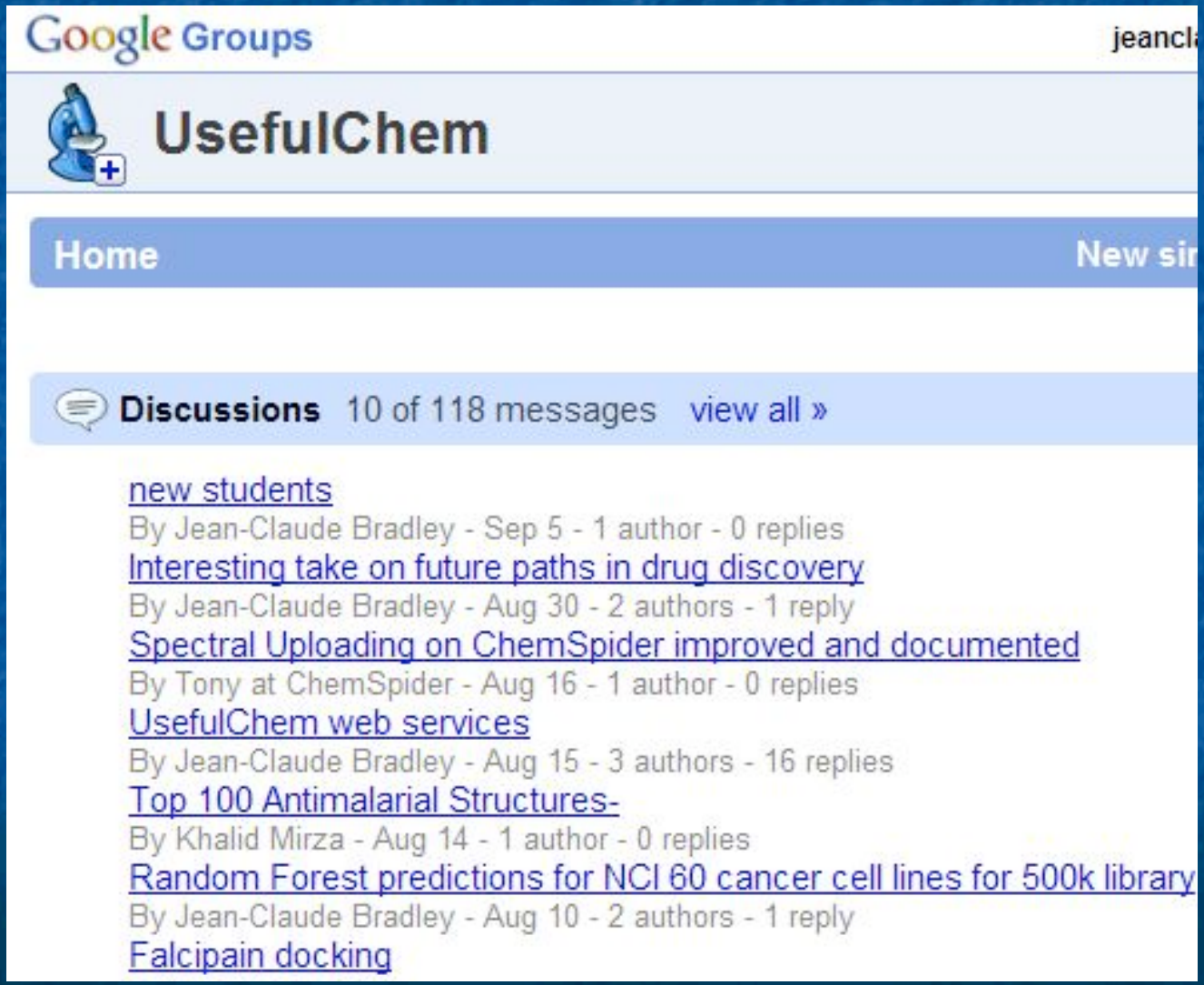
The following are successful experiments to make DOPAL:

1. EXP016 (2006-06-28) **jgiammarc/Lin (crude)**
2. EXP023 **Khalid (crude)**
3. EXP025. **(2006-08-31) Khalid/Lin (pure without chromatography)**

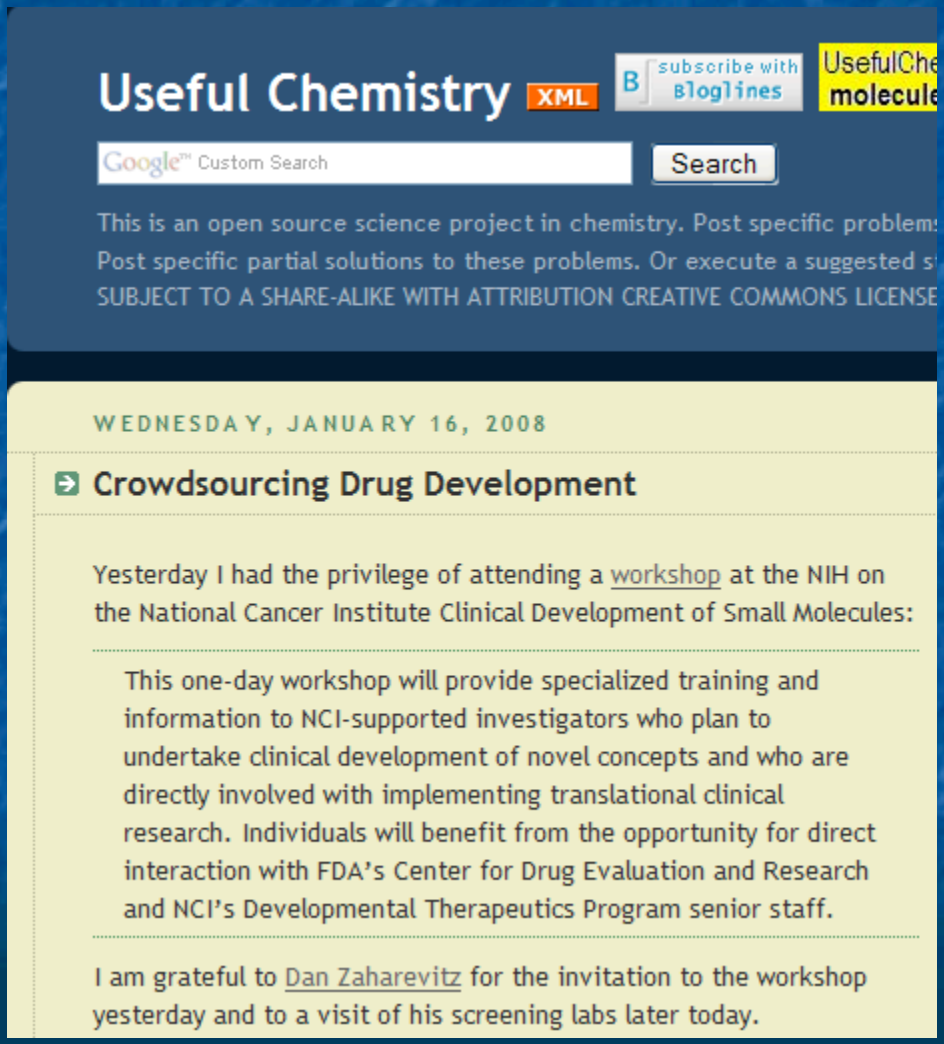
The story of the failures that made the success possible:

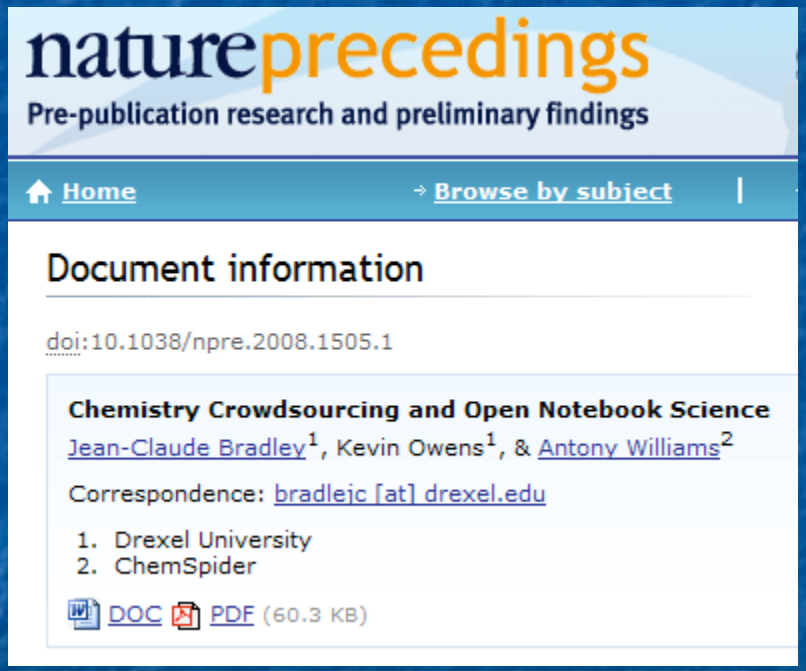
Our initial attempts focused on modifying a report of the decomposition of adrenaline in glacial acetic/perchloric acids in order to avoid using perchloric acid. With limited access to NMR for a few months, we attempted to monitor the progress of the reaction mainly by TLC. Based on reported purification of DOPAL

Mailing List Facilitates inter-group collaboration

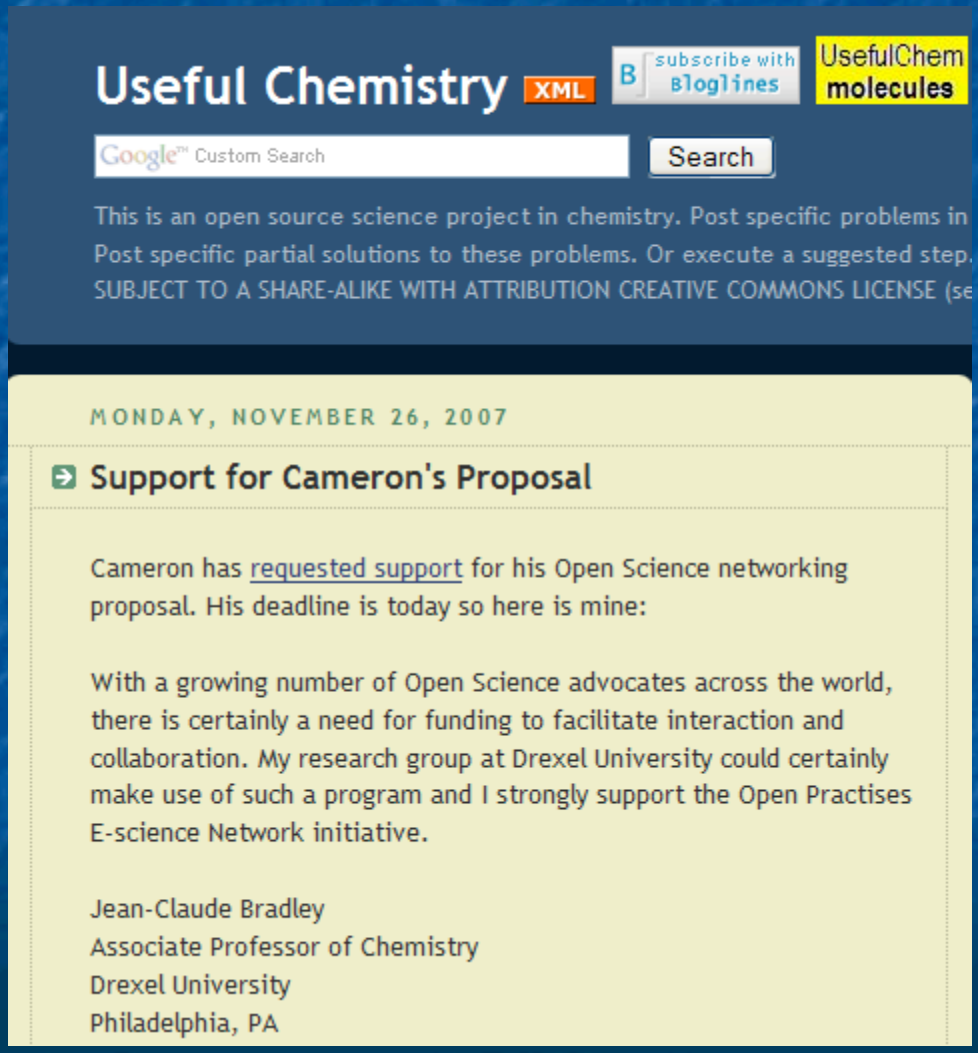


What about the blog? Discussing Funding





Supporting Funding Initiatives



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MONDAY, NOVEMBER 26, 2007

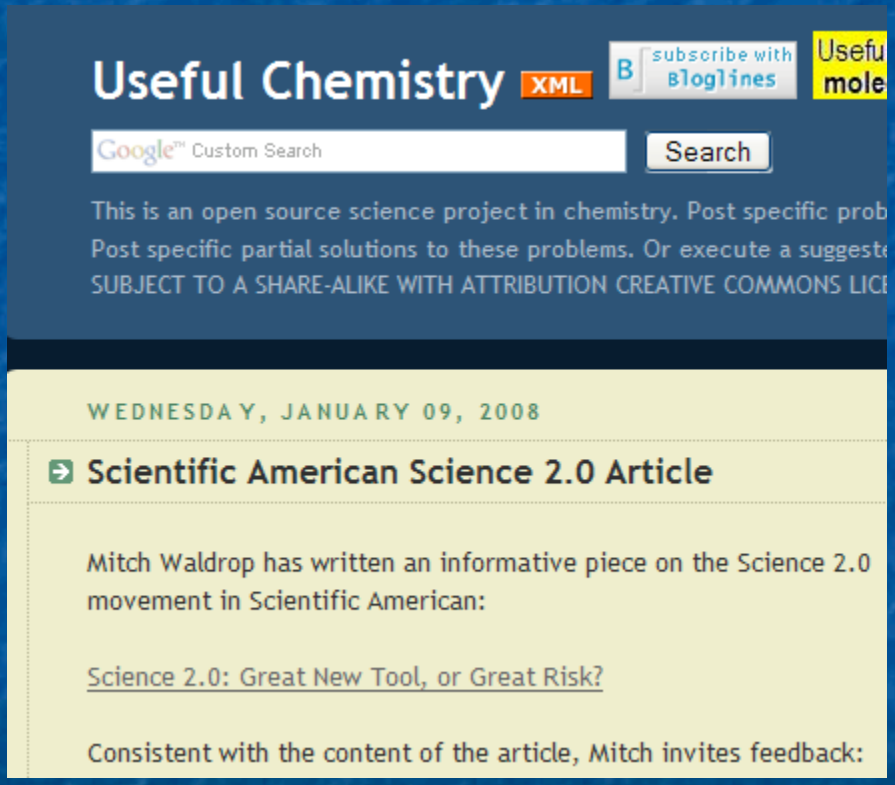
Support for Cameron's Proposal

Cameron has requested support for his Open Science networking proposal. His deadline is today so here is mine:

With a growing number of Open Science advocates across the world, there is certainly a need for funding to facilitate interaction and collaboration. My research group at Drexel University could certainly make use of such a program and I strongly support the Open Practises E-science Network initiative.

Jean-Claude Bradley
Associate Professor of Chemistry
Drexel University
Philadelphia, PA

Highlight Popular Media Coverage



SCIENTIFIC AMERICAN

Highlight Peer-Reviewed Coverage

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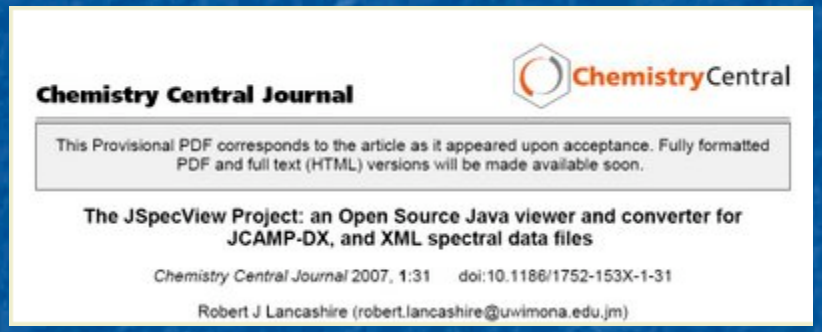
SATURDAY, DECEMBER 08, 2007

JSpecView Article on Chemistry Central

Robert Lancashire has just published an article in Chemistry Central Journal:

The JSpecView Project: an Open Source Java viewer and converter for JCAMP-DX, and XML spectral data files

Our lab has found this software to be key for communicating organic chemistry results within an Open Notebook Science environment. All NMR raw data and metadata are automatically recorded and users from anywhere can mine the spectra by expanding and integrating at will from a browser interface. This is an enormous improvement over the traditional method of storing and publishing spectra as images that cannot be expanded.



Chemistry Central Journal

ChemistryCentral

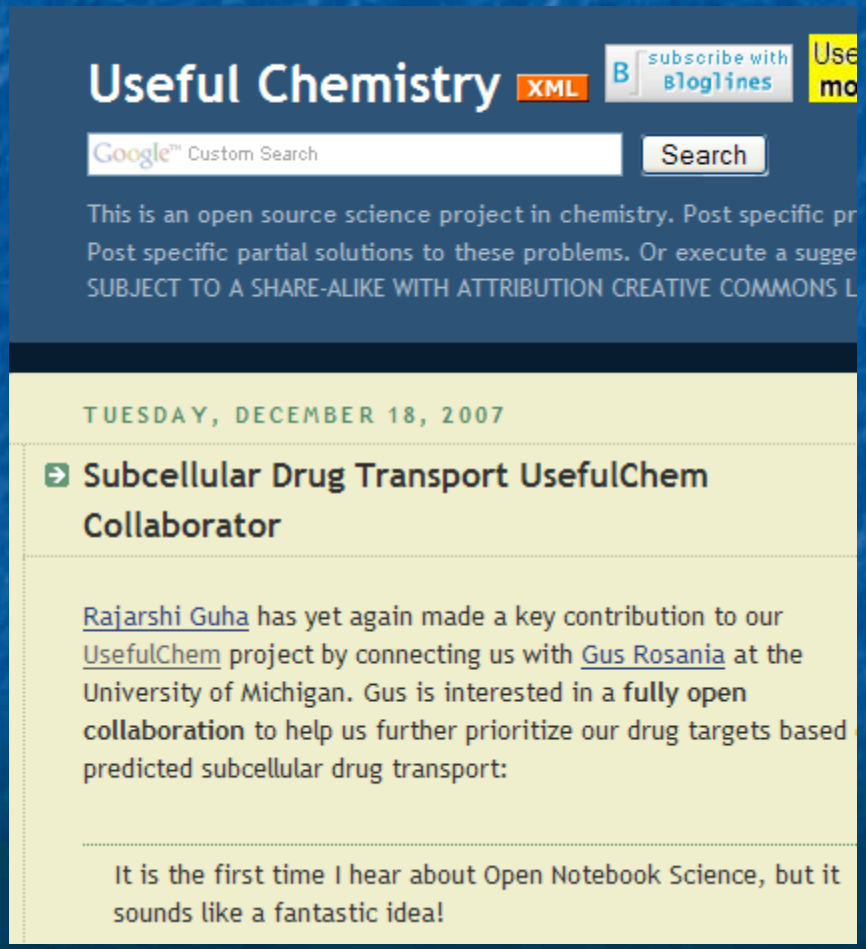
This Provisional PDF corresponds to the article as it appeared upon acceptance. Fully formatted PDF and full text (HTML) versions will be made available soon.

The JSpecView Project: an Open Source Java viewer and converter for JCAMP-DX, and XML spectral data files

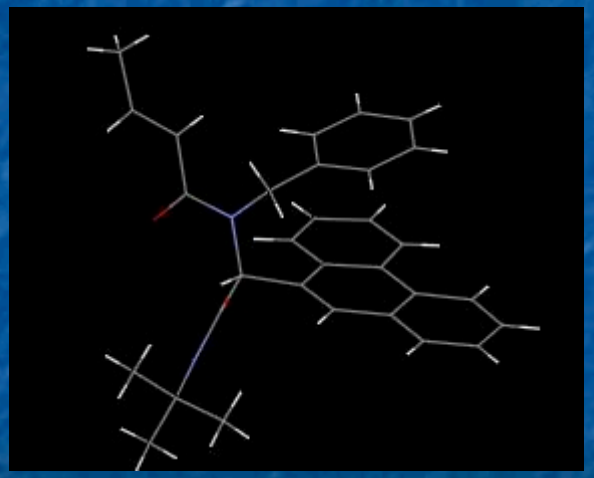
Chemistry Central Journal 2007, 1:31 doi:10.1186/1752-153X-1-31

Robert J Lancashire (robert.lancashire@uwimona.edu.jm)

Announce Collaborator: Gus Rosania



Announce Collaborator: Matthias Zeller



Announce Collaborator: Phil Rosenthal

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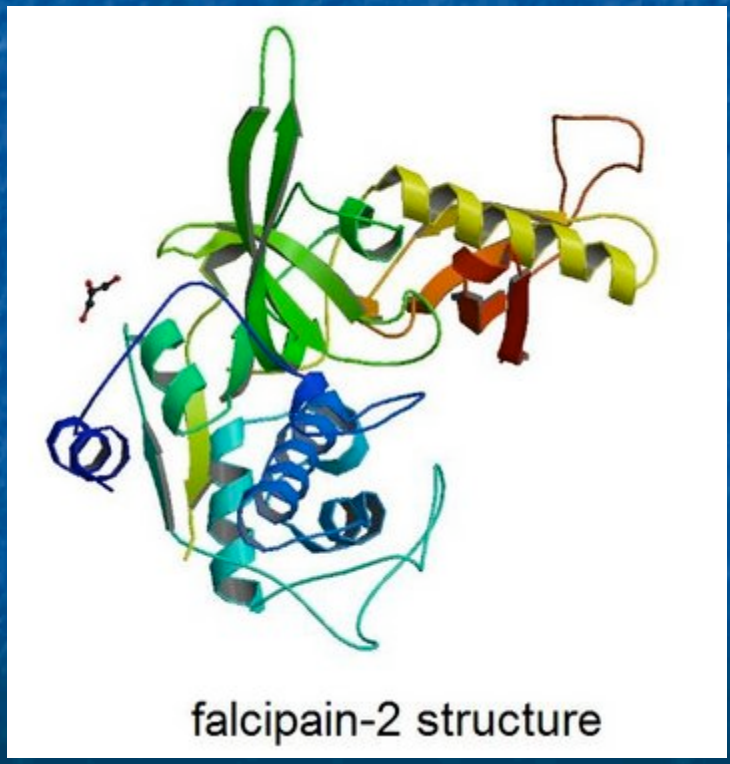
WEDNESDAY, AUGUST 08, 2007

Falcipain Collaboration

Thanks to Barry Bunin of Collaborative Drug Discovery, we now have a collaborator who will run assays on the compounds from our CombiUgi project. We'll be using our account on CDD to manage the activity results.

Phil Rosenthal from UCSF has agreed to run assays on the inhibition of falcipain-2, an enzyme used by the malaria parasite to digest hemoglobin. As described in UCSF magazine, the Rosenthal group discovered the enzyme and have developed an assay.



falcipain-2 structure

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THURSDAY, NOVEMBER 29, 2007

Swarthmore Talk on Open Notebook Science

On Tuesday November 27, 2007 I had the pleasure of speaking at Swarthmore on our UsefulChem project and Open Notebook Science more generally.

Liz Evans and Cheryl Grood from the Swarthmore Sigma Xi Chapter did a wonderful job in rounding up people to have discussions both before and after my talk at dinner. This gave us an opportunity to share teaching experiences with new technologies (blogs, wikis, Second Life, etc.) - something I didn't really get into too deeply during my talk.

Drexel CoAS talks mp3 podcast

subscribe with Bloglines transcript

Wednesday, November 28, 2007

Swarthmore Sigma Xi ONS Talk

On November 27, 2007 I presented our work on Open Notebook Science. I had a little more time to explain most aspects of our work to a scientific, but not necessarily a chemistry audience.

Near the end I did discuss some of our very recent results relating to our CombiUgi project and the synthesis of some compounds about to to be tested for the inhibition of the malarial parasite's enzyme Falcipain-2.

Here is the audio (mp3)
Here is the Flash screencast.
Here is the Powerpoint.

Discuss Presentations in Second Life

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TUESDAY, OCTOBER 16, 2007

Science Bloggers SFLO Session

Berci led yesterday's (Oct 15, 2007) SciFoo Lives On session on Science Bloggers.

Sandra Porter, Bora Zivkovic and I (UsefulChem) discussed why and how we blog about science.
Bora really had a lot of problems with his video card and I was impressed that he persisted to deliver a great presentation and participate. I've been there so I know how frustrating that can be. Unfortunately a lot of people assume that is the typical Second Life experience and give up.

Berci live blogged the event here and did a tremendous job in representing the flow of the session. The transcript and other links are here.

Showcase Science in New Media

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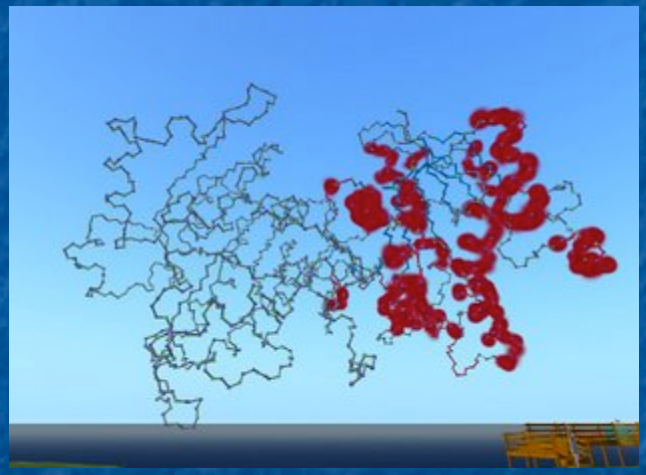
TUESDAY, DECEMBER 04, 2007

More Proteins in Second Life

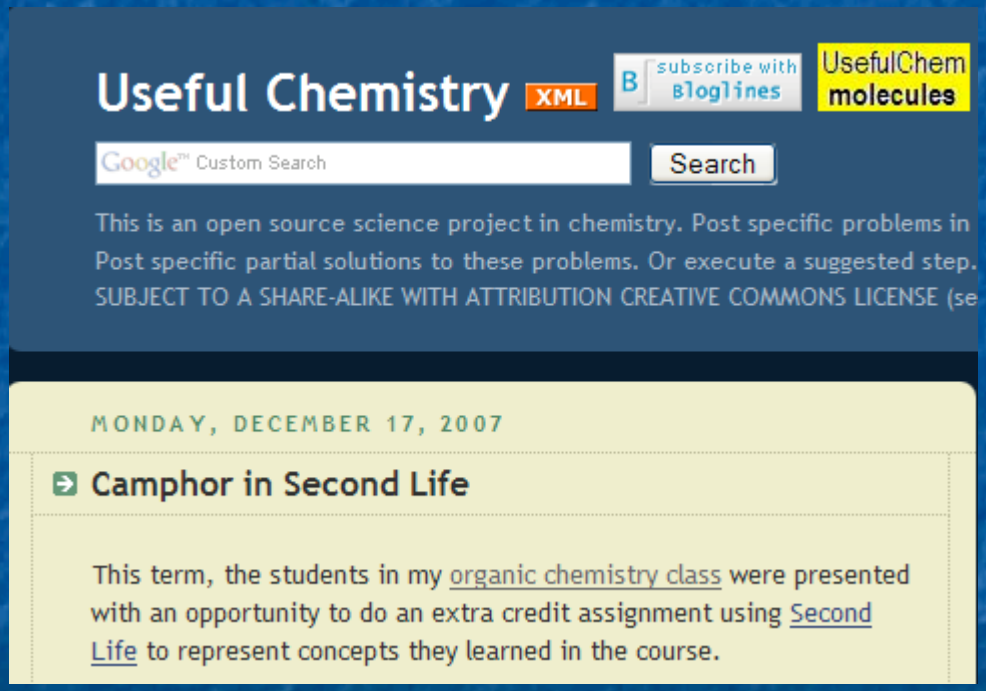
For those of you following chemistry in Second Life, take a look at Peter Miller's Tidal Blog.

Peter has been posting a lot lately about rendering proteins in Second Life. For example, here is malarial enoyl reductase, an enzyme that has been a target of the UsefulChem group for some time.

Although we did demonstrate the docking of a molecule in a pocket of enoyl reductase, it is nice to see the whole enzyme.



Showcase Teaching in New Media



Alerts to Broader Impact Opportunities

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THURSDAY, DECEMBER 06, 2007

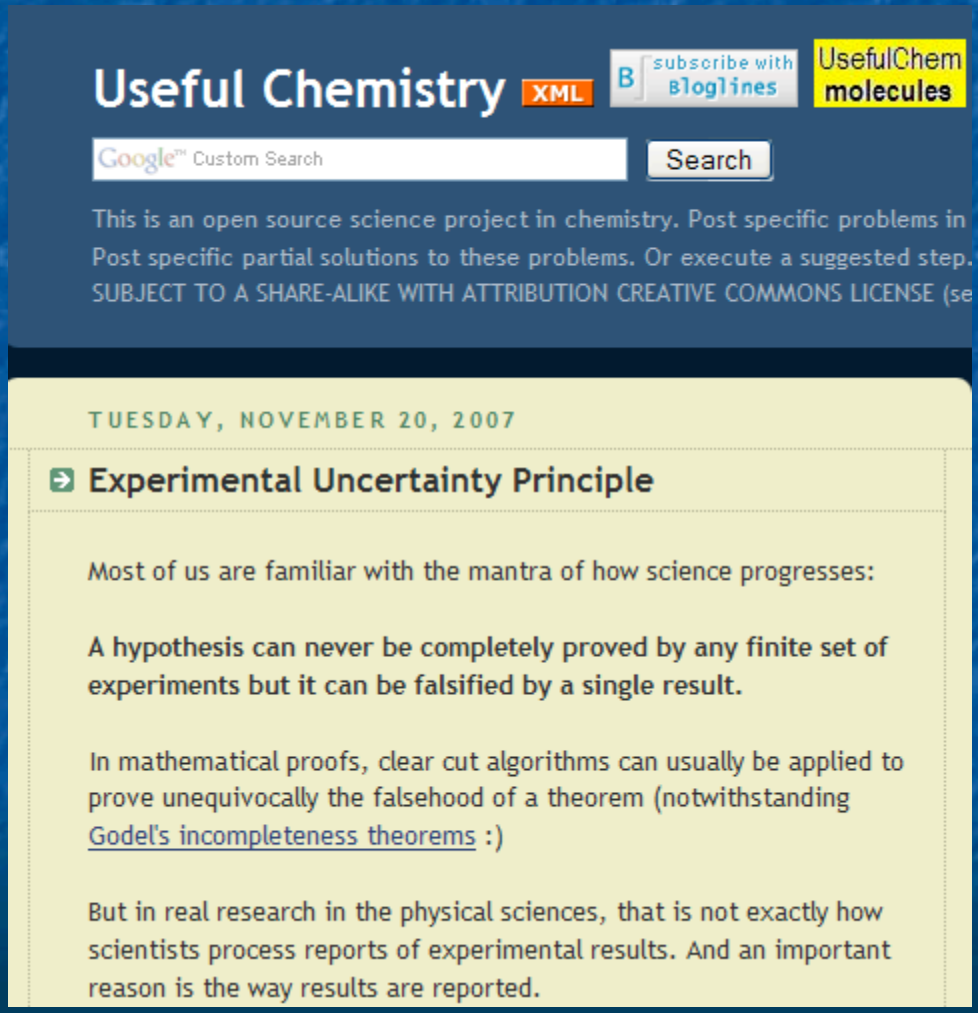
Run for Malaria in Philly

For anyone in the Philadelphia area who cares about malaria:

Drexel University Crossings Stair Run

Beta Beta Beta and the Office of Residential Living will sponsor a stair run Saturday, December 8, 2007, from 9 a.m. to noon in University Crossings (101 N. 32nd Street).

Science Philosophy



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TUESDAY, NOVEMBER 20, 2007

Experimental Uncertainty Principle

Most of us are familiar with the mantra of how science progresses:

A hypothesis can never be completely proved by any finite set of experiments but it can be falsified by a single result.

In mathematical proofs, clear cut algorithms can usually be applied to prove unequivocally the falsehood of a theorem (notwithstanding Godel's incompleteness theorems :)

But in real research in the physical sciences, that is not exactly how scientists process reports of experimental results. And an important reason is the way results are reported.

Gus Rosania's Notebook

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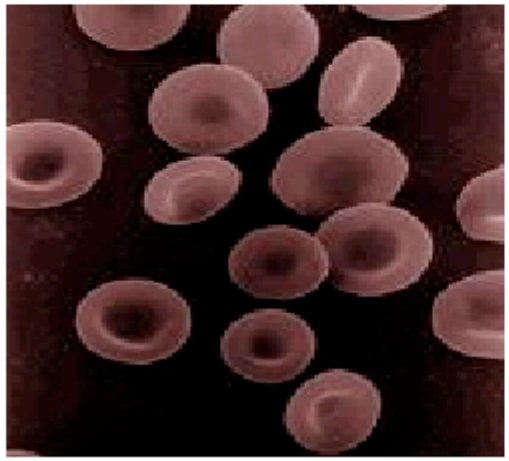
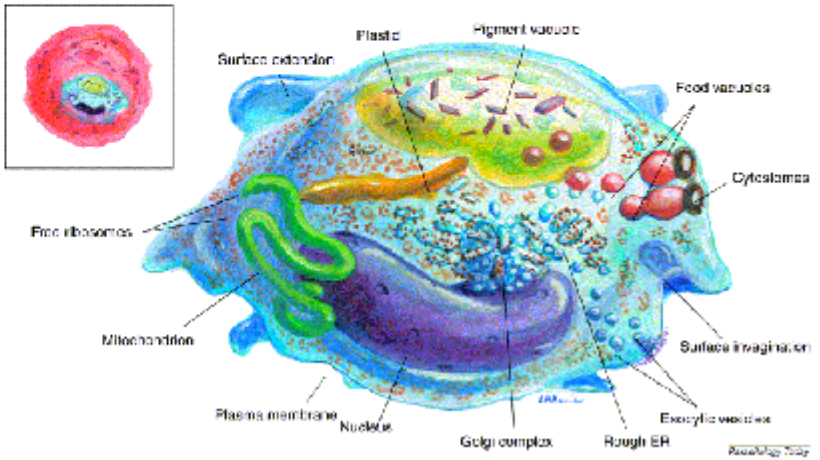
Virtual cell 4.4 beta version.

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





Collaboration with Brent Friesen's Teaching Lab

CHEM254 An OpenScience Collaboration: Exploring the Ugi Reaction

"Ugi to the left, Ugi to the right. This is so fun, we're gonna Ugi all night."

The UsefulChem Project:
This experiment represents the beginning of collaboration with the UsefulChem Bradley open notebook science group of undergraduate research at Drexel University.[1] The goal of the UsefulChem project is to use the Ugi 4 component reaction to synthesize possible anti-malarial compounds. Open notebook science allows immediate dissemination of experimental results that invites advice and suggestions as well as complementary experiments that enhance and advance the project. We are going to reproduce some of the Drexel results as well as perform two complementary reactions that have not been done at Drexel.

Cameron Neylon's Notebook

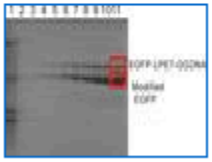
Sortase Cloning

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.

Where is Science headed?