Education 2.0: Leveraging Collaborative Tools for Teaching

E-Learning 2.0 Conference at Drexel University

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Education 2.0

Web 2.0 Tools Applied to Education

A Web 2.0 site allows its users to interact with other users or to change website content, in contrast to non-interactive websites where users are limited to the passive viewing of information that is provided to them.

http://en.wikipedia.org/wiki/Web_2.0

So many tools … so little time

CMS (e.g. Blackboard)

recorded lectures (e.g. podcasts, screencasts, videos)

blogs

games

clickers

free course content (e.g. OpenCourseWare)

free online textbooks

wikis

virtual worlds (e.g. Second Life)

Principle of Highest and Best Use

Highest and best use is a concept in real estate appraisal. It states that the value of a property is directly related to the use of that property. This use, the Highest and Best Use, may or may not be the current use of the property.

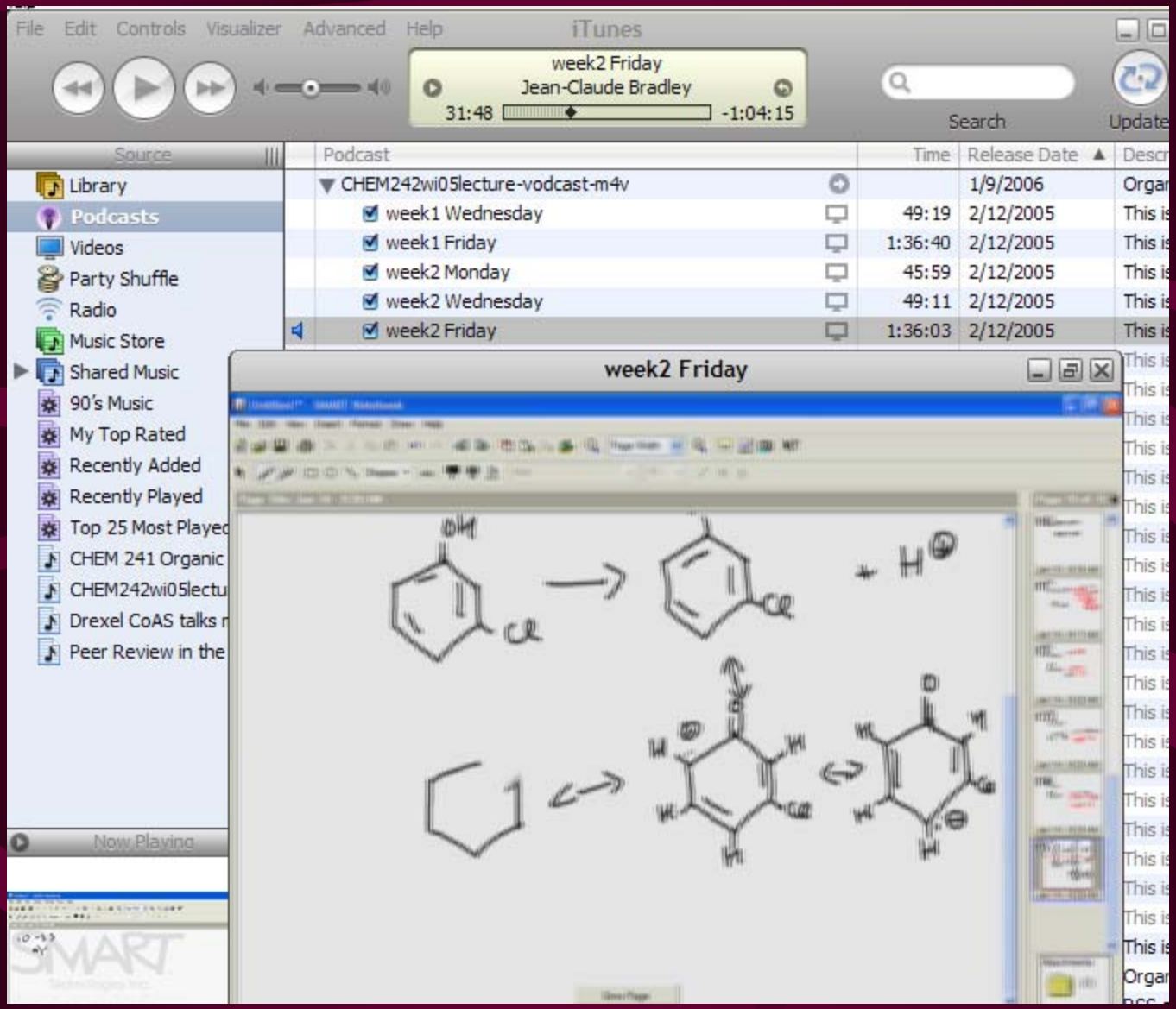
What is the best use of your time as a teacher?

- **Lecturing?**
- **Manual grading?**
- **Discussion groups?**
- **Posting to a blog?**
- **Motivating?**

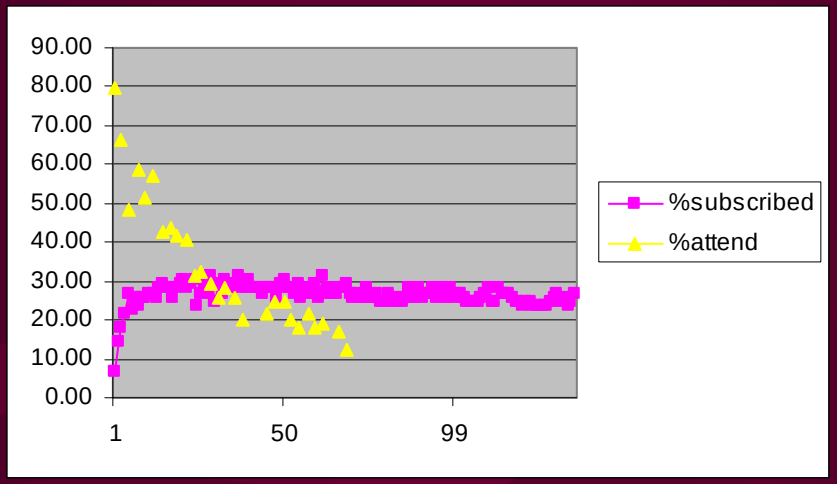
What are your objectives?

- **Increasing the baseline understanding of the average student?**
- **Helping the best students actualize their potential?**

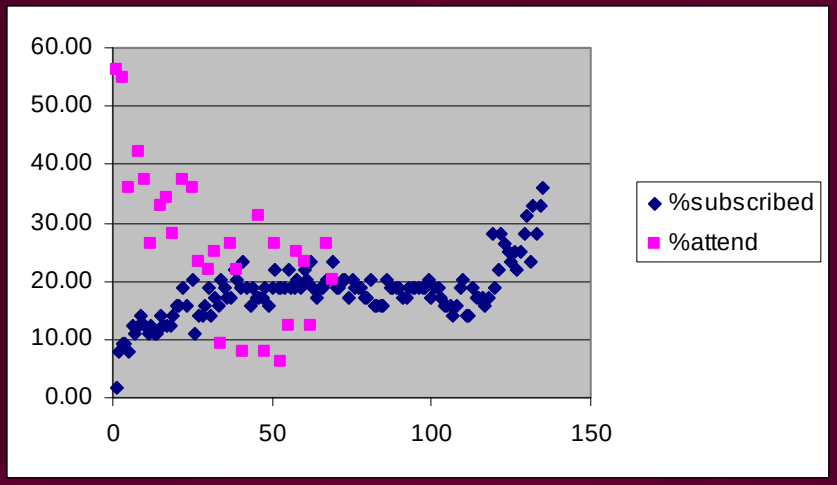
Screencasting: easy solution for recording lectures



Natural migration from F2F to screencast/podcast channels



CHEM 241
89 students



CHEM 243
64 students

Best use of Class Time

Mainly repeating lectures

Mainly workshops

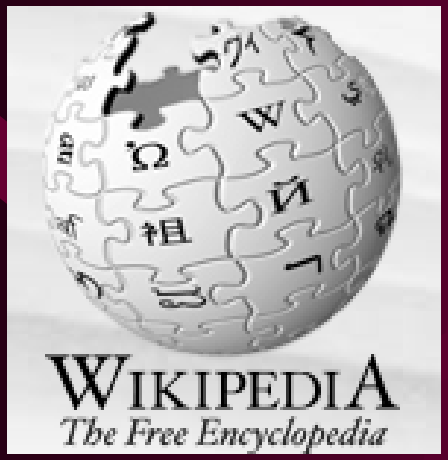
One-on-one mentoring

Doing problems

Games

Wikis

A wiki is a website that allows the easy creation and editing of any number of interlinked web pages via a web browser using a simplified markup language or a WYSIWYG text editor.

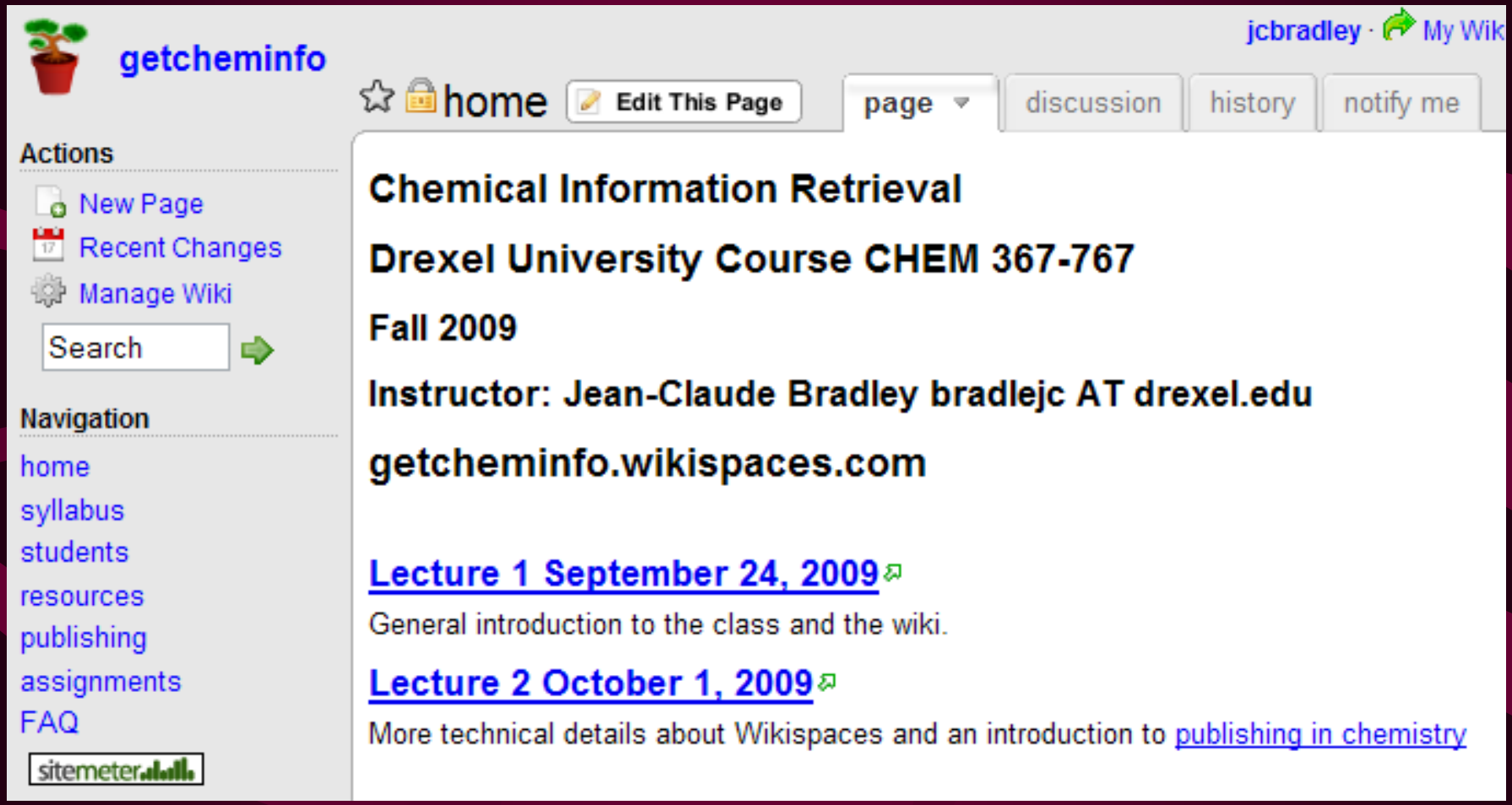


http://en.wikipedia.org/wiki/Wiki

Educational Uses of Wikis

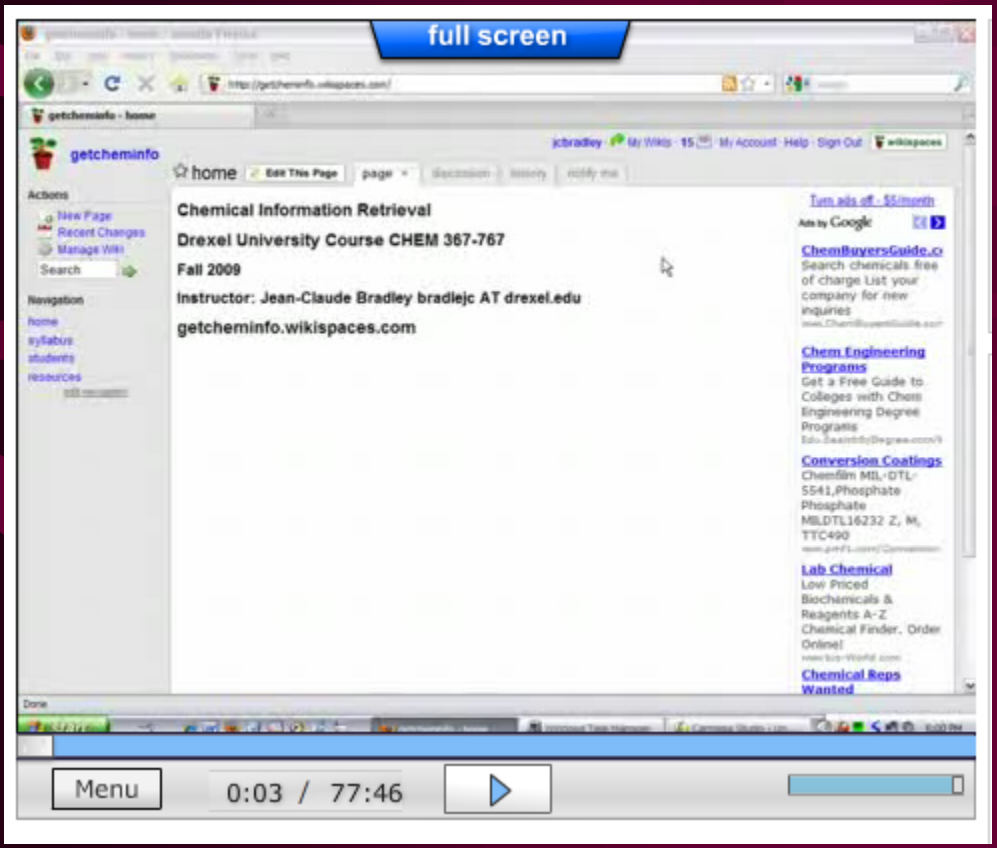
- Organizing course content
- Student assignments
- Student generated content
- Easy to make content public and rapidly indexed on Google

Example: Chemical Information Retrieval FA09 (CHEM367/767)



Use of Web2.0 Tools for Sharing Recorded Lectures

SciVEE™ beta — Making science visible



Chemical Information Retrieval class 1 FA09

by: jcbradley | September 25, 2009

Jean-Claude Bradley introduces Chemical Information Retrieval (CHEM 367 and CHEM 767) at Drexel University with an overview of topics to be covered. See class wiki at http://getcheminfo.wikispaces.com for details. « Hide

Info | Share | Flag this video

640 views | DOI: 10.4016/12845.01 | login to rate

Comments

You must be logged in to comment

Students participate to collect resources

Resources

Multi-media/creative component tools

AcaWiki Make comprehensive summaries of selected papers you read.

RasMol Make slick models of complex molecular systems (see example of lipid bilayer).

Services

Interlibrary Loans ILL service

Databases

Compilations

Precompetitive preclinical ADME/Tox data (Ekins and Williams)

List of Free Chem Databases by Rich Apodaca

Free

ChemSpider

Google

WolframAlpha

Wikipedia

Orgsyn

Assignments

Assignments

1. Write a summary of one of the articles you are reading for your project paragraph by paragraph. One or two sentences per paragraph is fine. You must do this in your own words. No significant amount of text can be copied from the abstract or any part of the paper. Either put the summary in bullet form on your research log or on AcaWiki. **Due November 5, 2009 20:50 PM**
2. Answer one of the FAQ questions or create and answer an FAQ question relating to a topic relating to chemistry publishing. You must provide at least one relevant reference. You must summarize in your own words - copying text from anywhere verbatim is not allowed. If all the questions have been answered create a reasonable one on some aspect of chemistry publishing not yet asked. **Due November 5, 2009 20:50 PM**
3. Find 5 independent sources of 5 properties associated with a molecule of your choice. Provide all references. (see jcblog as an example of the format) **Due November 12, 2009**

Article summaries on Web2.0 site

AcaWiki

Democratization of Academic Knowledge...

page discussion edit edit source history

Evaluation of ultra performance liquid chromatography Part I Possibilities and limitations

Citation: *André de Villiersa, François Lestremaub, Roman Szucsb, Sylvie Gélébartb, Frank Davida, Pat Sandra (2006/09) Evaluation of ultra performance liquid chromatography Part I Possibilities and limitations. Journal of Chromatography A (Volume 1127) (RSS)*

doi: 10.1016/j.chroma.2006.05.071

Student Research Logs: DMT

☆ Adam Myers LOG | Edit This Page | page | discussion | history | notify me

Adam Myers
Endogenous alkaloids
[You'll have to narrow this down but definitely a good place to start JCB]

9/1/09- What functions does endogenous dimethyltryptamine play in humans. **[Perfect scope JCB]**
The Hallucinogen N,N-Dimethyltryptamine (DMT) Is an Endogenous Sigma-1 Receptor Regulator
-sigma 1 receptor regulator
Endogenous psychoactive tryptamines reconsidered: an anxiolytic role for dimethyltryptamine
[wow - that is a really interesting article - I would like to learn more about the TA receptors JCB]
-anxiolytic
-neurotransmitter at the TA (Trace Amine) system
-biosynthesis from tryptophan

http://getcheminfo.wikispaces.com/Adam+Myers+LOG

Green Tea Project

☆ Jose Rafael Quejada LOG | Edit This Page | page | discussion | history | notify m

Does Green Tea increase Longevity?
09/25/09
Green tea has:

- polyphenols
- catechins (more specifically epigallocatechin gallate)
- carotenoids
- tocopherols
- ascorbic acid
- chromium
- manganese
- selenium
- zinc

source: wikipedia.com
interesting articles via web of science link:
Polyphenolic Chemistry of Tea and Coffee: A Century of Progress
Green tea and bone metabolism
Green tea consumption and gastric cancer in Japanese: a pooled analysis of six cohort studies

Inhibitory effects of epigallocatechin-3 gallate, a polyphenol in green tea, on tumor-associated endothelial cells and endothelial progenitor cells

My plan right now is to:
-find an article supporting the wikipedia page claims **[Excellent start - also try substructure searches for some of your compounds]**

http://getcheminfo.wikispaces.com/Jose+Rafael+Quejada+LOG

Chemistry of Chocolate

October 5, 2009

Thinking about doing my research paper on something more interesting like...CHOCOLATE!! Something like "Is Chocolate Really Addicting?"

But I think that topic may be too general.

So, I did a primary search on what some researchers think makes chocolate so addicting.

I learned that the answer isn't so short and simple.

Found article on ScienceDirect:

"Chocolate: Food or Drug?"

"Most likely, a combination of chocolate's sensory characteristics, nutrient composition, and psychoactive ingredients, compounded with monthly hormonal fluctuations and mood swings among women, will ultimately form the model of chocolate cravings."

I looked at another book written by Astrid Nehlig (two Ph.D. degrees in physiology and functional neurochemistry) called Coffee, Tea, Chocolate, and the Brain.

In her book, she talks about certain drug-like substances in chocolate, such as phenylethylamine and methylxanthines.

It seems really interesting and I would like to look over it, too.

[This would make for a very interesting report - if you can resolve the conflicting reports about phenylethylamine by carefully reading the primary literature JCB]

http://getcheminfo.wikispaces.com/Sarah+Shim+Log

Students generate course content

Chemical Information Retrieval FAQ

instructions

Bill Hooker suggested the OAD site for ideas on questions you may wish to answer

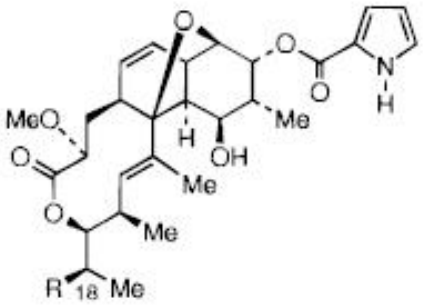
1. What are primary, secondary and tertiary sources?

A primary source is the source of information. In other words, the primary source will give you more information than anything else one would be able to find. Primary sources can a journal article, lab notebook, or patent. For instance, the lab notebook used to record the data of the experiment performed or the published results of that experiment would be primary sources for that experiment. A secondary source, on the other hand, is not the source of information but rather analyzes and talks about information from other sources, usually primary sources. A common example of a secondary source is a review article. Lastly, a tertiary source is similar to a secondary source in that it analyzes and talks about information from other sources. In addition, tertiary sources generalize and summarize information from primary and/or sources. Examples of tertiary sources include encyclopedias and Wikipedia.

References:

"Primary, Secondary and Tertiary Sources." *PORT: Penn Online Research Tutorial*. 15 October 2009. <http://gethelp.library.upenn.edu/PORT/sources/primary_secondary_tertiary.html>

Students curate data on ChemSpider



1, R = OH, nargenicin A_1
3, R = H, 18-deoxynargenicin A_1

- **[Nick Paparoidamis]**
- Smiles: C[C@@H](O)[C@H]2OC(=O)[C@H](C[C@H]1C=CC5[C@H]4O[C@]1(C(C)=C[C@H]2C)[C@@H]5[C@H](O)[C@@H](C)[C@H]4OC(=O)c3cccn3)OC
- nargenicin
- Article found from Scifinder
- The closest chemspider ID for nargenicin is 4885360. In chemspider, not all the stereocenters are specified. This article has the exact stereochemistry of nargenicin for every stereocenter in the compound.
- The stereostructure of nodusmicin was established by X-ray crystallographic studies, while that of nargenicin A1 was confirmed by its synthesis from nodusmicin. The absolute configuration of the nargenicins, originally assigned by Cane by the nonempirical CD exciton method, was subsequently verified via Kallmerten's enantioselective total synthesis of (+)-18-deoxynargenicin A1 (3).

[Approved by ChemSpider JCB]

Five Sources for the solubilty of EGCG

In addition, the amount of caffeine extracted from green and black tea was greater than the amount of EGCG. This is due to the difference in water solubility and molecular weight between EGCG and caffeine. The water solubility of caffeine is 21.7 g/L, while that of EGCG is about 521.7 g/L.

of specific isolation of caffeine from fresh tea leaf. Water solubility of caffeine is 21.7 g l^{-1} while that of EGCg, the most important component of tea catechins, is about 5 g l^{-1}. The molecular weight of caffeine is 194.2 while

http://usefulchem.blogspot.com/2010/01/dangerous-data-lessons-from-my-cheminfo.html

WTF?!

Specification Sheet

SIGMA-ALDRICH

Product Name	(−)-Epigallocatechin gallate, ≥95%, from green tea
Product Number	E4143
Product Brand	SIGMA
CAS Number	989-51-5
Molecular Weight	458.37
Storage Temp	2-8°C

TEST	SPECIFICATION
APPEARANCE	WHITE TO FAINT PINK POWDER
SOLUBILITY	CLEAR FAINT YELLOW OR FAINT PINK SOLUTION AT 5MG/ML IN WATER

sample	solubility in water[a] (mM)
EGCG	5.12 ± 2.21

=2.3 g/L

http://usefulchem.blogspot.com/2010/01/dangerous-data-lessons-from-my-cheminfo.html

The End of the Chain of Provenance

Water Solubility Analysis. All excess EGCG and EGCG glycosides were mixed in 200 μL of water in an Eppendorf tube, at room temperature. A 3510R-DTH ultrasonic cleaner (Branson, Danbury, CT) was used to maximize solubility. After 1 h of sonication at room temperature, each of the samples was diluted and then filtered through a 0.45 μm MFS membrane (Adventec, Pleasanton, CA) for HPLC analysis, to determine the concentrations. A model 1525 HPLC system, connected to a 400 × 3.9 mm i.d. μ-Bondapak C_{18} column (Waters, Milford, MA) and a model 2487 UV detector (Waters) at 280 nm were utilized to quantify the amounts of EGCG and EGCG glycosides. The mobile phase consisted of 23% methanol and was conducted via the isocratic method, with a flow rate of 0.5 mL/min. The concentrations of the EGCG and EGCG glycosides were calculated as was described previously by Li et al. (*19*).

http://usefulchem.blogspot.com/2010/01/dangerous-data-lessons-from-my-cheminfo.html

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

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

Motivation: Faster Science, Better Science

There are NO FACTS,
only measurements embedded within assumptions

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

TRUST

PROOF

Crowdsourcing Solubility Data

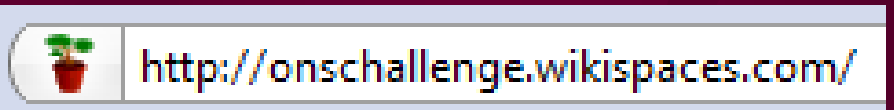
Open Notebook Science Challenge

Sponsors

Submeta Open Notebook Science Awards - Apply Here

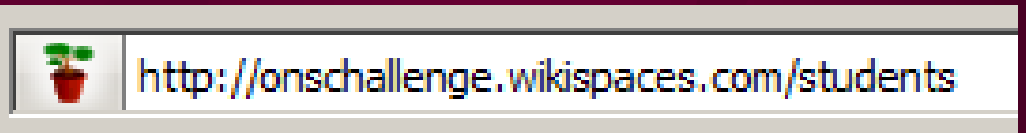
What?

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



ONS Submeta Award Winners

1. **December 2008: Jenny Hale**
2. **January 2009: Khalid Mirza**
3. **February 2009: David Bulger**
4. **March 2009: Cedric Tchakounte**
5. **April 2009: Tim Bohinski**
6. **June 2009: Matthew Federici**
7. **July 2009: Marshall Moritz**
8. **August 2009: Daniel Rein**
9. **September 2009: Jenna Mancinelli**
10. **December 2009: Hai Truong**



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

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

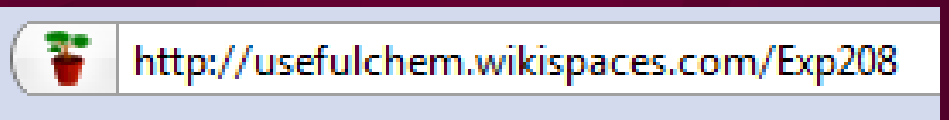
12:30 Solvent twas added to appropriate vials from which solvent had evaporated- All the vials had been capped tight (flip top) (***- next time get pic at this stage***)
13:20 Samples were vortexed again, until no more of the solid would dissolved..the vortex time varied from few seconds to about 7min, 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

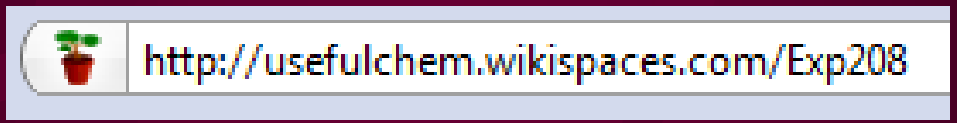
The values for 4-chlorobenzaldehyde are very low in all solvents, including chloroform.--HNMR This is due to the prolonged time left in the speed-vac and the volatility of this aldehyde. Boiling point of 4-chlorobenzaldehyde at 1 atm. is 213-215 C (*Chemspider*) and the boiling point at 0.1 Torr is calculated 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-chlorobenzaldehye 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 compunds (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

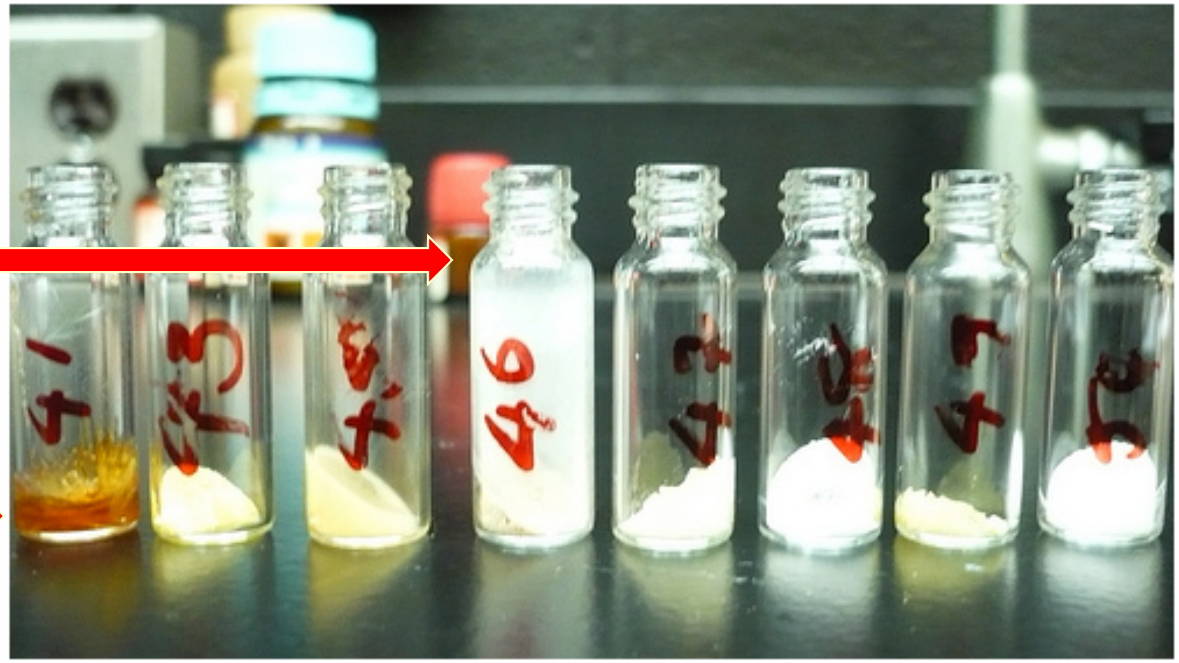
flickr

Splatter?

Some liquid

Usefulchem EXP208 41b-50b

ALL SIZES



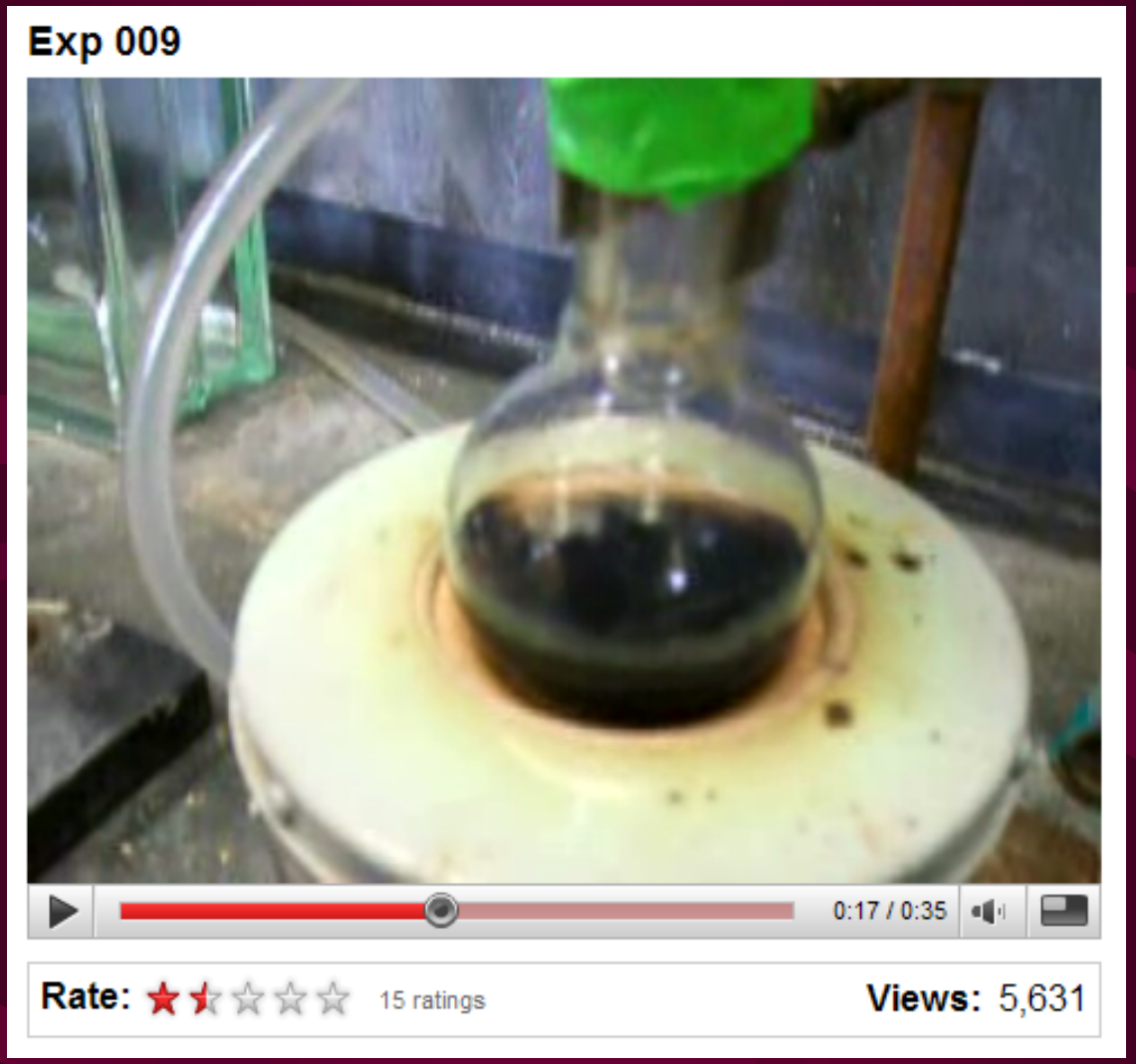
Comments

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



Calculations Made Public on Google Spreadsheets

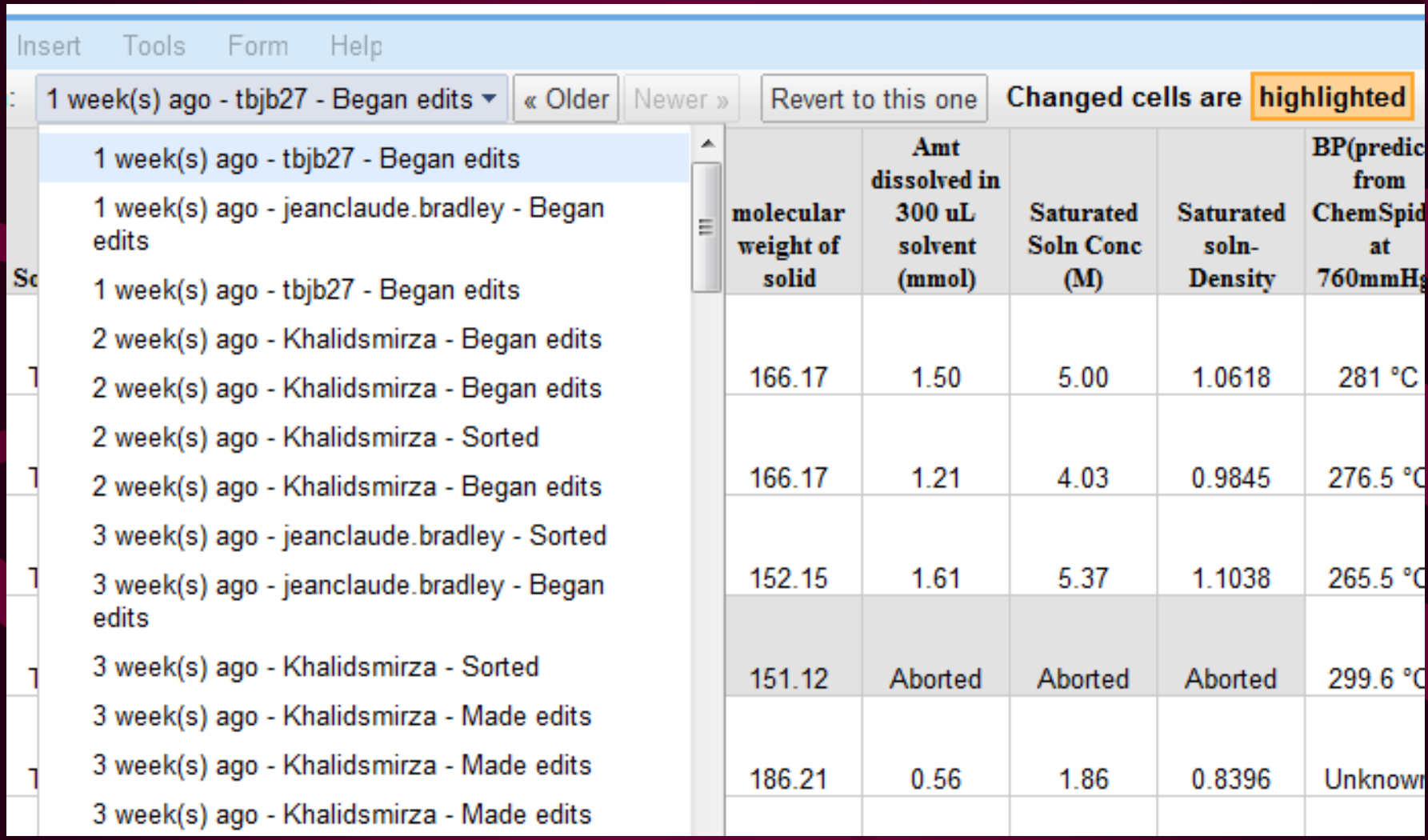
EXP208-WS1

File Edit Format Insert Tools Form Help

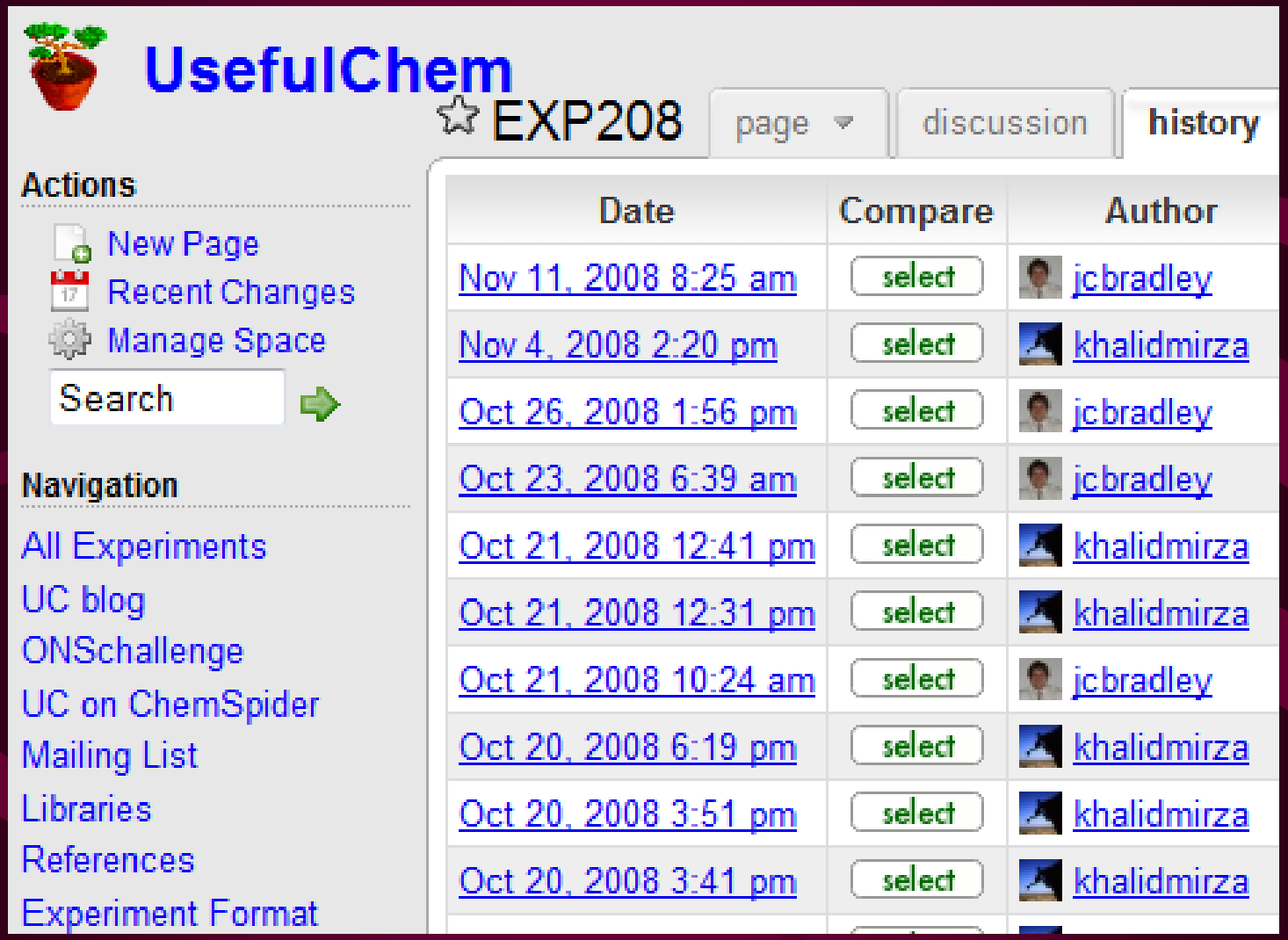
	A	B	C	D	E	F	G	H	I	J	K	L	M
	Si	ID	Solute	Solvent	Wt of empty vials (g)	Wt of vial w/solution (300uL)	Wt of sample solution (300uL)	Wt of vial after SpeedVac (g)	Solid dissolved in 300 uL of solvent (mg)	molecular weight of solid	Amt dissolved in 300 uL solvent (mmol)	Saturated Soln Conc (M)	Saturated 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

http://usefulchem.wikispaces.com/Exp208

Revision History on Google Spreadsheets



Wiki Page History



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-chlorobenzaldehye 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 compunds (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.

Solubilities collected in a Google Spreadsheet

Google Docs

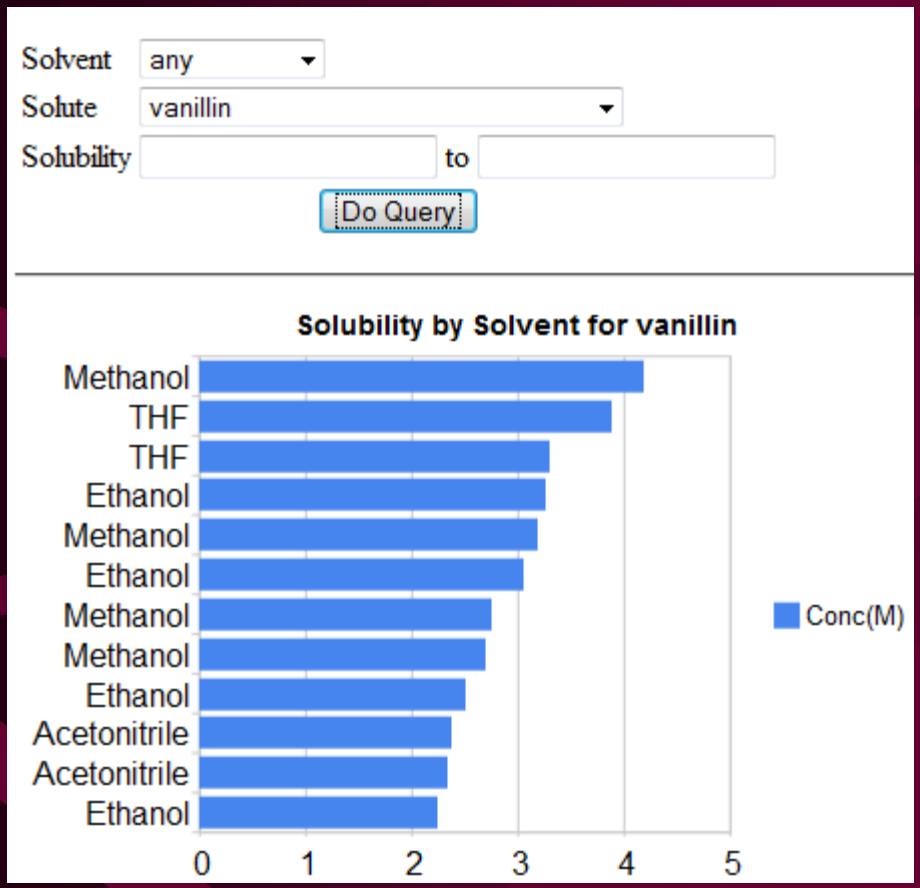
SolubilitesSum

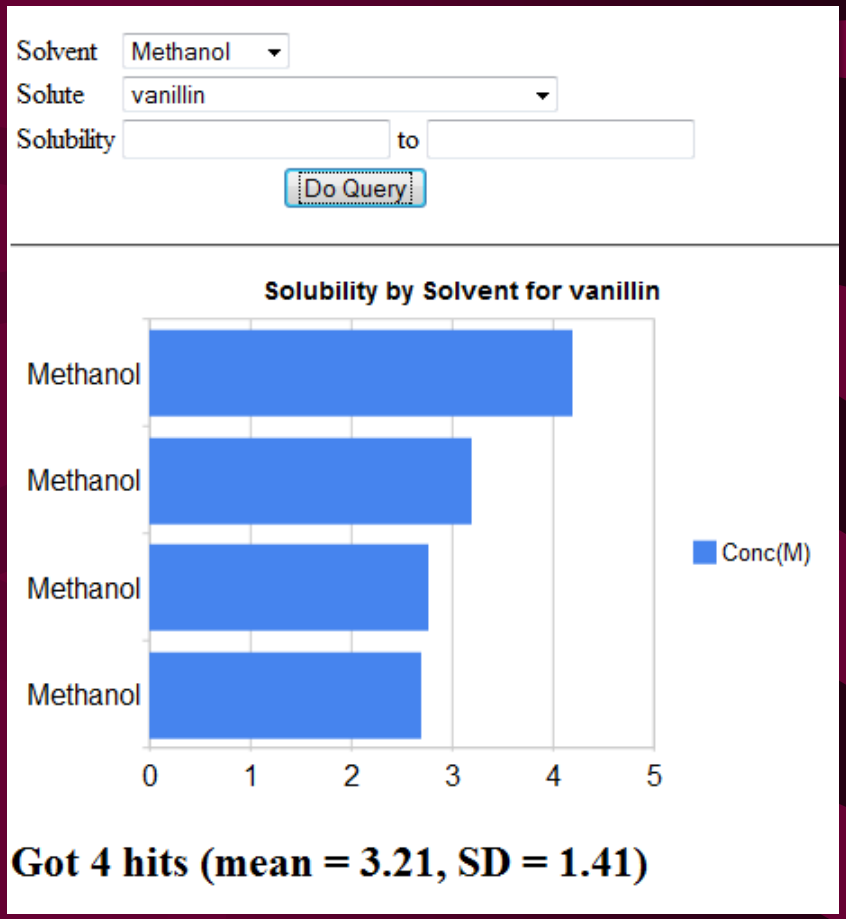
File Edit Format Insert Tools Form Help

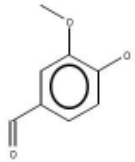
	A	B	C	D
	EXP	sample	ref	solute
2	208	11b	http://usefulchem.wikispaces.com/exp208	3,4-dimethoxybenzaldehyde
3	208	41b	http://usefulchem.wikispaces.com/exp208	3,4-dimethoxybenzaldehyde
4	208	21b	http://usefulchem.wikispaces.com/exp208	3,4-dimethoxybenzaldehyde
5	208	3b	http://usefulchem.wikispaces.com/exp208	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
COc1cc(ccc1OC)C=O	Acetonitrile	N#CC	5.57	UC	
COc1cc(ccc1OC)C=O	Ethanol	OCC	5.55	UC	
COc1cc(ccc1OC)C=O	Chloroform	ClC(Cl)Cl	5.44	UC	
Oc1c(cccc1OC)C=O	THF	O1CCCC1	5.37	UC	
COc1cc(ccc1OC)C=O	THF	O1CCCC1	5.00	UC	
COc1cc(ccc1OC)C=O	Methanol	OC	4.92	UC	
O=C(O)/C=C/C	Ethanol	OCC	4.65	UC	
O=C(O)/C=C/C	Methanol	OC	4.56	UC	
O=C(OC(C)(C)C)NCC(=O)O	Methanol	OC	4.40	UC	YES

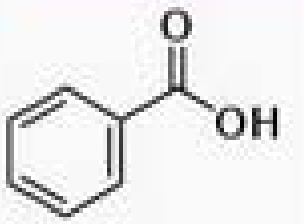
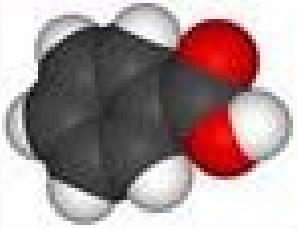
Rajarshi Guha's Live Web Query using Google Viz API





Serial	EXP	Sample	Ref	Solute	Solute SMILES	Solvent	Solvent SMILES	Conc (M)
1	207	3	http://usefulchem.wikispaces.com/exp207	vanillin		Methanol	OC	4.19

Data provenance:
From Wikipedia to...

Benzoic acid	
	

Properties	
Molecular formula	C_6H_5COOH
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

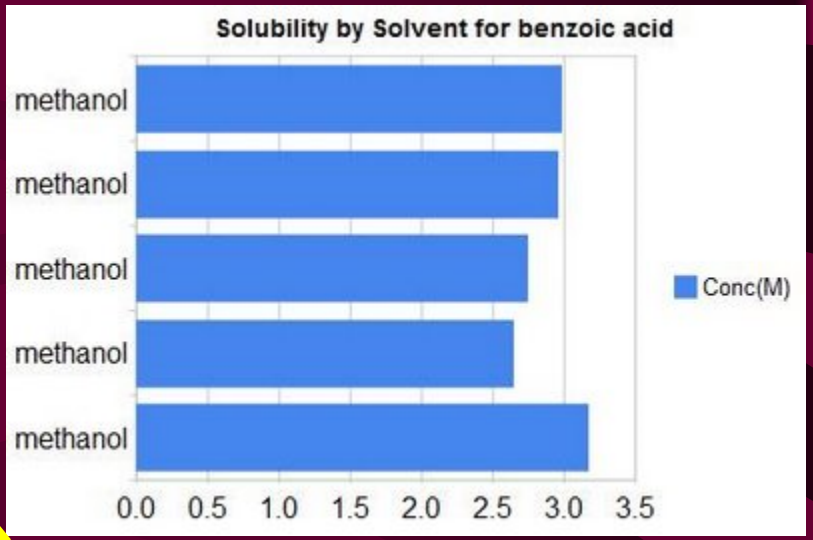
1. ^ http://oru.edu/cccda/sl/solubility/allsolvents.php?solute=benzoic%20acid Open Notebook Science Challenge Data.

...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). Fo
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 po
saturation. Each vial is vortexed for 30 seconds. After the process of vortexing is complet
centrifuged for one minute. 300µl of the mother liquor is then pipetted into pre-weighed ha
solution is weighed and entered into the speedvac, noting the pressure,. The solution is th
of 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

http://www.lulu.com/content/paperback-book/8337972

Open Notebook Science Challenge: Solubilities of Organic Compounds in Organic Solvents (3RD)

by Andrew Lang et al.

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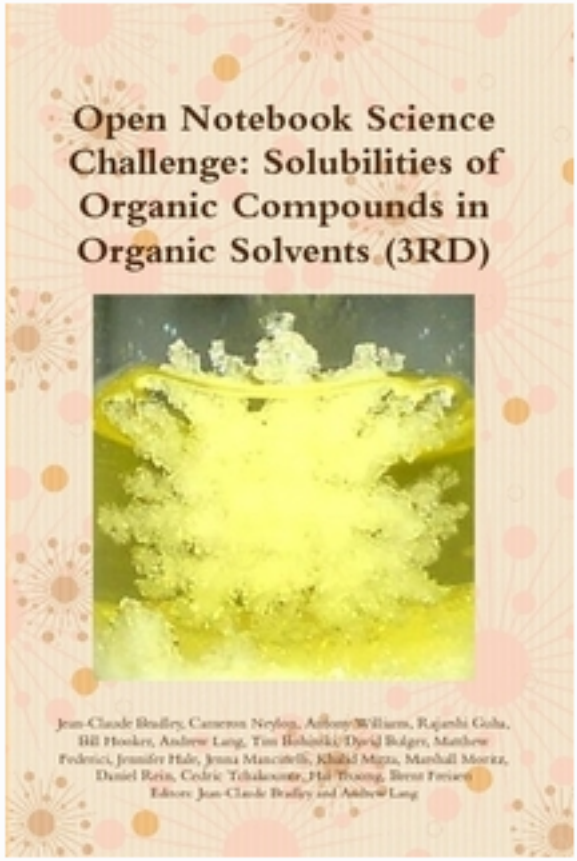

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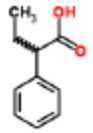
Solubilities of organic compounds in organic solvents compiled and measured during the Open Notebook Science Challenge

Product Details

ISBN	978-0-557-31801-8
Copyright	©2010 Jean-Claude Bradley, et al.
Language	English
Country	United States
Publication Date	February 11, 2010
Page Count	130 pages
Size	U.S. Trade
Binding	Perfect Bound
Interior Color	Black And White



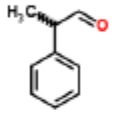
Compound Data

Molecular weight	164.201	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.38
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.09 g/cm³
SMILES	O=C(O)C(c1ccccc1)CC				
InChIKey	OFJWFSNDPCAWDK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	ppb (g/100g)
acetonitrile	6.18	0.83	1968.04
DMSO	5.97	0.81	886.12
ethanol	6.20	0.85	1977.18
THF	5.96	0.82	1059.60
toluene	5.35	0.74	519.73

2-phenylpropanal $C_9H_{10}O$[21]



Compound Data

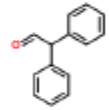
Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.13
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	0.98 g/cm³
SMILES	c1ccccc1C(C)C=O				
InChIKey	IQVAERDLDAZARL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	ppb (g/100g)
methanol	7.53	¤	¤

¤ Solute is very soluble/miscible, conversion fail.

2,2-diphenylacetaldehyde $C_{14}H_{12}O$[21]



Compound Data

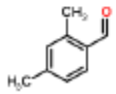
Molecular weight	196.245	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	3.67
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	1.069 g/cm³
SMILES	c1ccccc1C(c1ccccc1)C(=O)				
InChIKey	HLLGFGBLKOIZOM-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	ppb (g/100g)
methanol	5.64	¤	¤

¤ Solute is very soluble/miscible, conversion fail.

2,4-dimethylbenzaldehyde $C_9H_{10}O$[21]



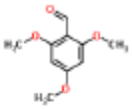
Compound Data

Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.56
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.003 g/cm³
SMILES	O=Cc1ccc(C)cc1C				
InChIKey	GISVICWQYMUPJF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	ppb (g/100g)
methanol	7.17	0.88	3128.10

2,4,6-trimethoxybenzaldehyde $C_{10}H_{12}O_4$[82]



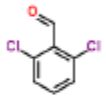
Compound Data

Molecular weight	196.2	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.49
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.133 g/cm³
SMILES	O=Cc1c(OC)cc(OC)cc1OC				
InChIKey	CRBZVDLXAIFERF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	ppb (g/100g)
THF	0.14	0.01	3.11

2,6-dichlorobenzaldehyde $C_7H_4Cl_2O$[208, 205]



Compound Data

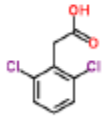
Molecular weight	175.012	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	3.03
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.4 g/cm³
SMILES	O=Cc1c(Cl)cccc1Cl				
InChIKey	DMIYKWPEFRFTPY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	ppb (g/100g)
acetonitrile	1.35	0.08	38.05
chloroform	3.41	0.32	69.35
ethanol	*	*	*
methanol	*	*	*
THF	2.48	0.22	69.58
toluene	1.74	0.19	44.68

* This aldehyde reacts with alcohols to form a hemiacetal.

2,6-dichlorophenylacetic acid $C_8H_6Cl_2O_2$[85, 82]



Compound Data

Molecular weight	205.038	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.71
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.456 g/cm³
SMILES	Clc1cccc(Cl)c1CC(=O)O				
InChIKey	SFAILOOQFZNOAU-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	ppb (g/100g)
THF	3.03	0.30	120.05

3-mercaptopropionic acid $C_3H_6O_2S$[22]

Compound Data

Molecular weight	106.144	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.43

Lulu.com Data Disks

http://www.lulu.com/content/compact-disc/8337307

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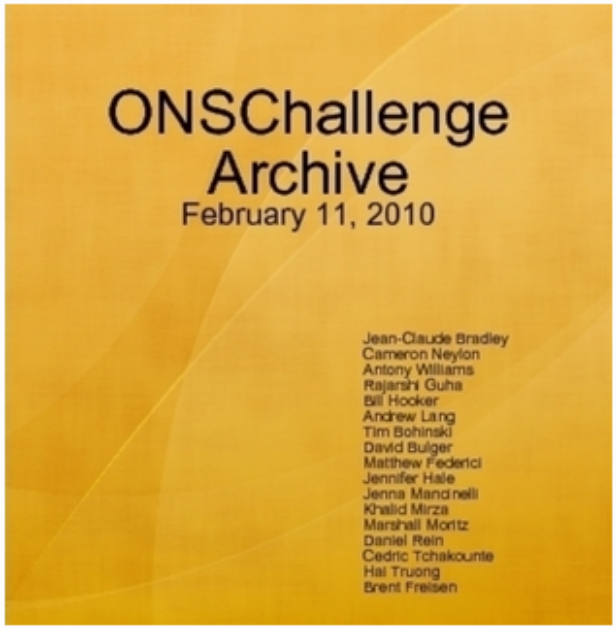

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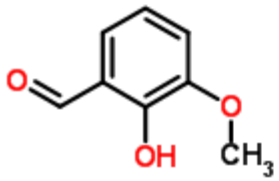
Inherent Properties, Identifiers and References

2D 3D



load save zoom

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

Systematic Name: 2-hydroxy-3-methoxy-benzaldehyde
SMILES: Oc1c(cccc1OC)C=O
InChI: InChI=1/C8H8O3/c1-11-7-4-2-3-6(5-9)8(7)10/h2-5,10H,1H3
InChIKey: JJVNINGBHGBWJH-UHFFFAOYAB

Names and Synonyms

Validated by Experts, Validated by Users,

205-715-3 *[EINECS/ELINCS]*
2-hydroxy-3-(methyloxy)benzaldehyde
2-Hydroxy-m-anisaldehyde
Benzaldehyde, 2-hydroxy-3-methoxy-
ortho-vanillin
o-Vanillin

Wikipedia Article(s)

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

Associated Data Sources and Commercial Suppliers

Data Source	
Alfa Aesar	A15672
ASDI	500011405
ChemPacific	

Predicted Properties

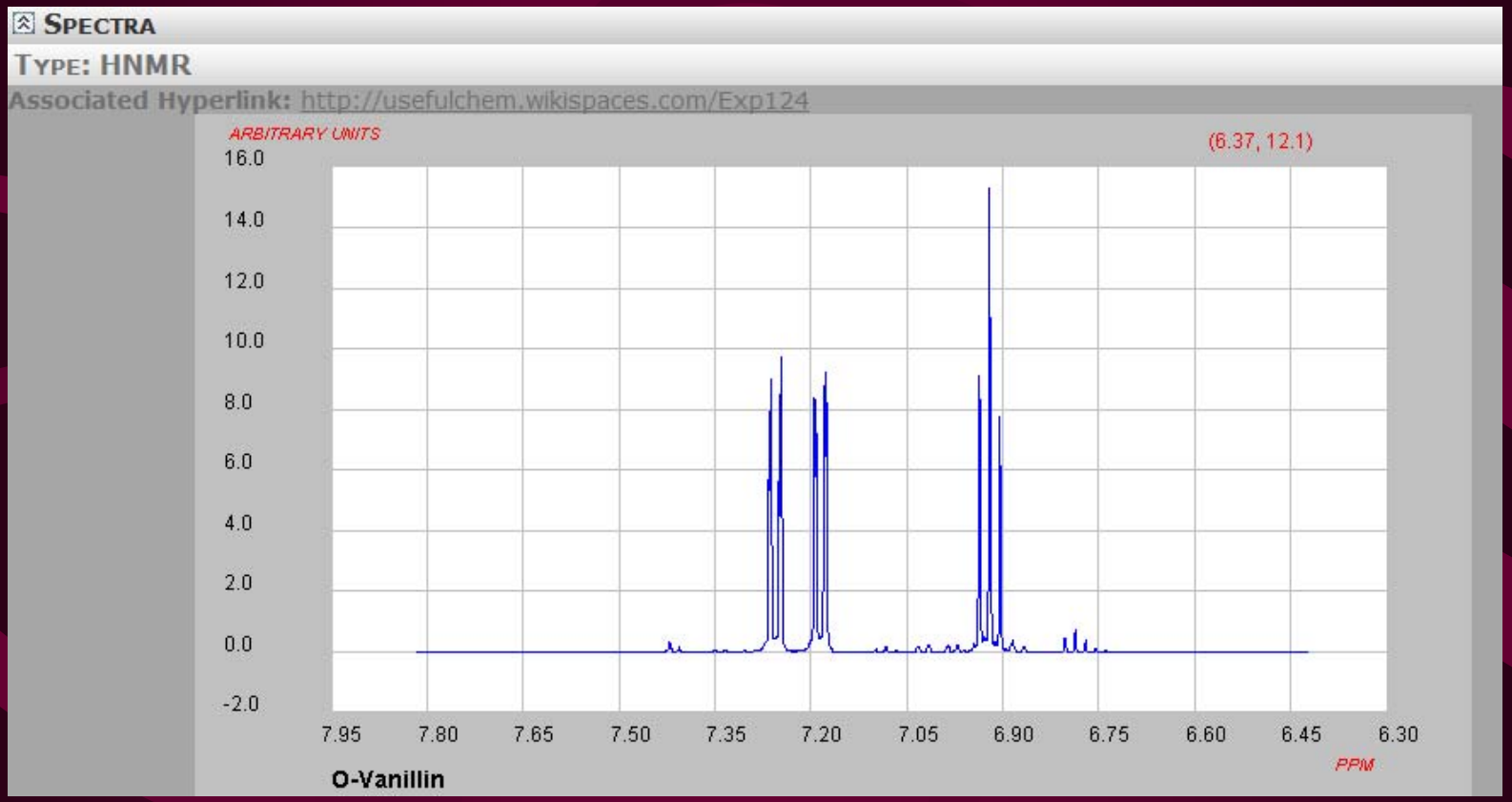
Boiling Point: 265.5 °C at 760 mmHg

Supplemental Information

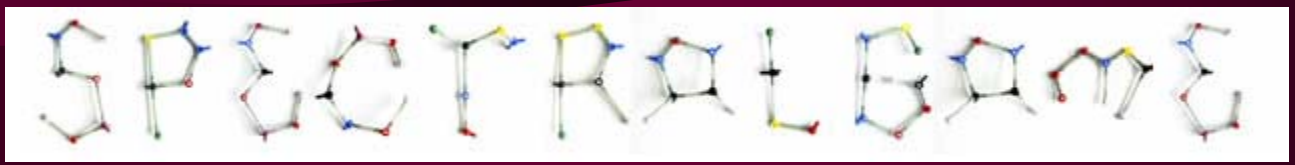
User Data

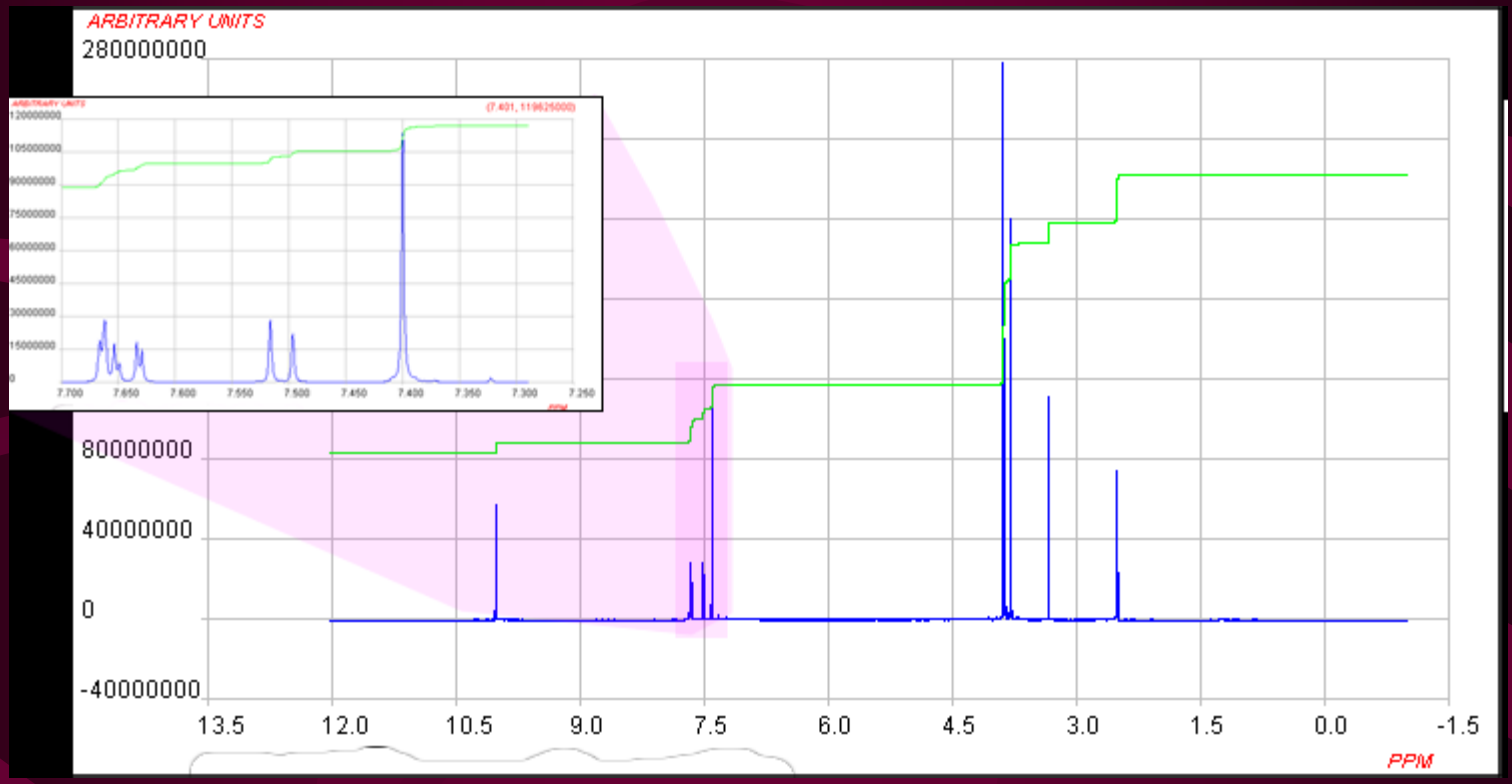
- **Experimental Physchem Properties**
  - **Melting Point:** 40-42
  - **Melting Point:** 40 - 42 C
  - **Boiling Point:** 265-266
  - **Boiling Point:** 265 C

User-Deposited Data on ChemSpider



Open Data JCAMP spectra for education



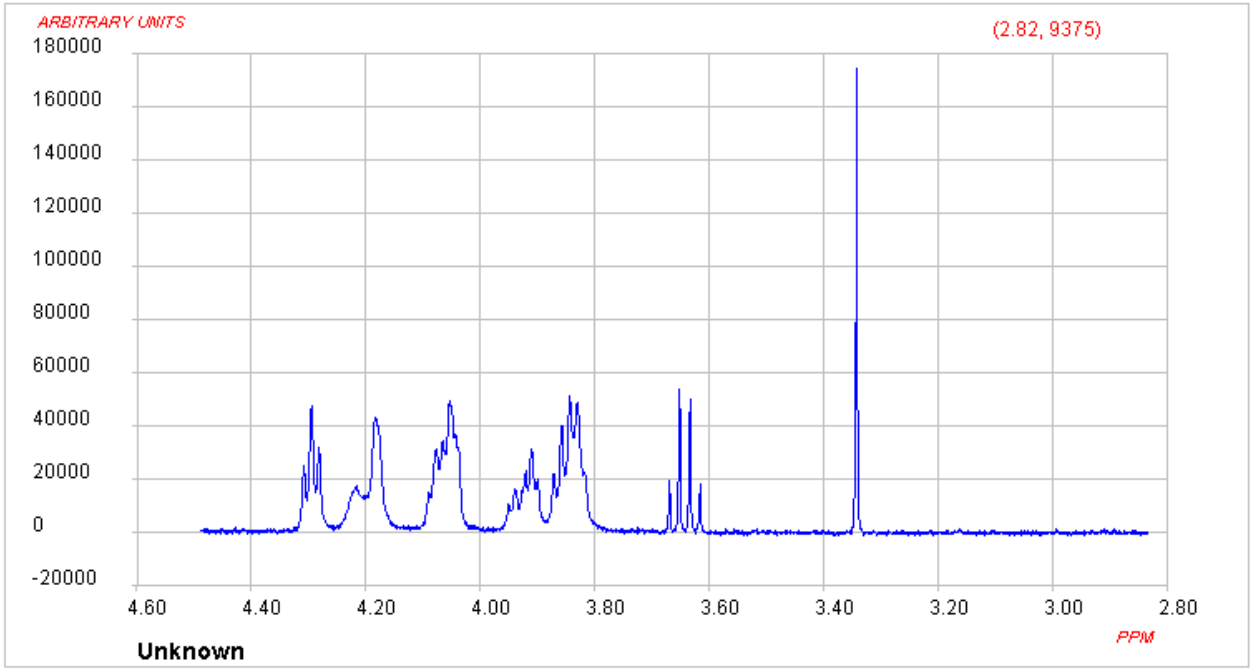


(Jean-Claude Bradley, Andy Lang, Tony Williams, Robert Lancashire)

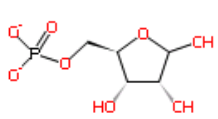
http://spectralgame.com/

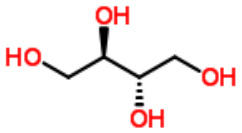
The game starts easy

Correct. Your Current Score: 1



Unknown





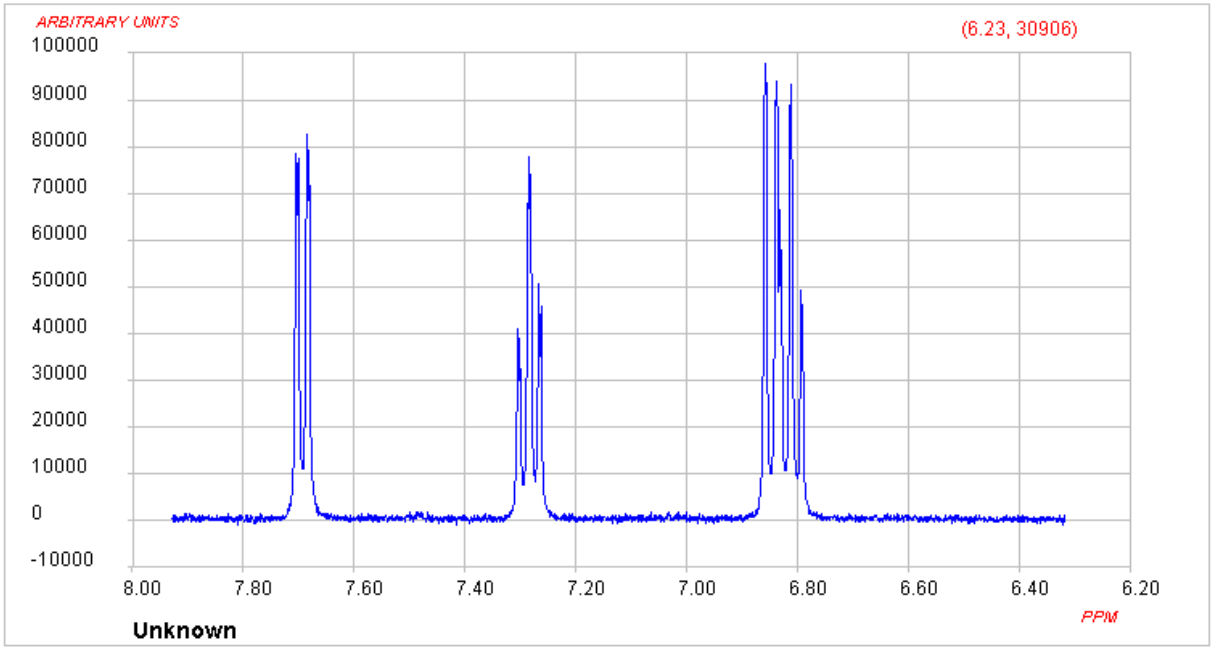
Click on the molecule that corresponds to the spectrum. Hit F11 to enlarge browser window.

No spectrum? Spectrum reversed? FLAG IT!

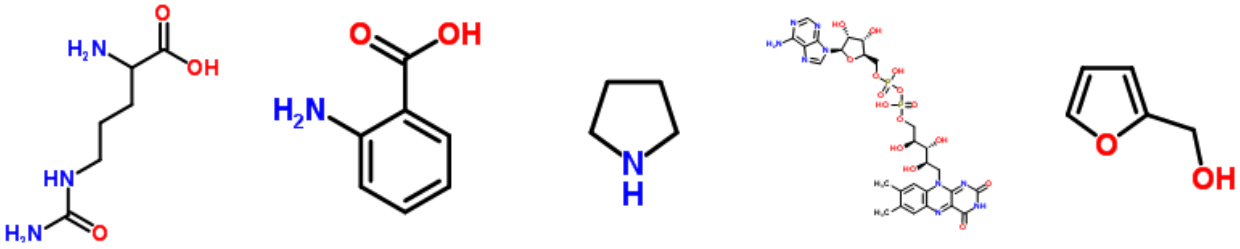
No spectrum? Something wrong with the spectrum? Comment. (opens in new window)

Later in the game: time limit and more molecules

Correct. Your Current Score: 40



Game Over in 27 seconds.



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)

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)

Flagged spectra get investigated

Link To Chemspider	Type	Times Correct	Times Incorrect	Percent Correct	Flagged	Comments
7811	HNMR	55	20	73		1
8640	HNMR	55	20	73	2	
17216135	HNMR	44	16	73		
76444	HNMR	58	21	73		
1152	HNMR	47	17	73	1	
21814	HNMR	50	18	74		
559198	HNMR	53	19	74	1	1
913						
82615						
1005						
467536						3
11542	HNMR	51	18	74		
21011	HNMR	37	13	74		
21428943	HNMR	37	13	74	1	1
553601	HNMR	57	20	74	1	

Comments

Chemispder Link - View Spectrum

Khalid says:

If this is trans-2-Pentenal..then the sample is way too impure.

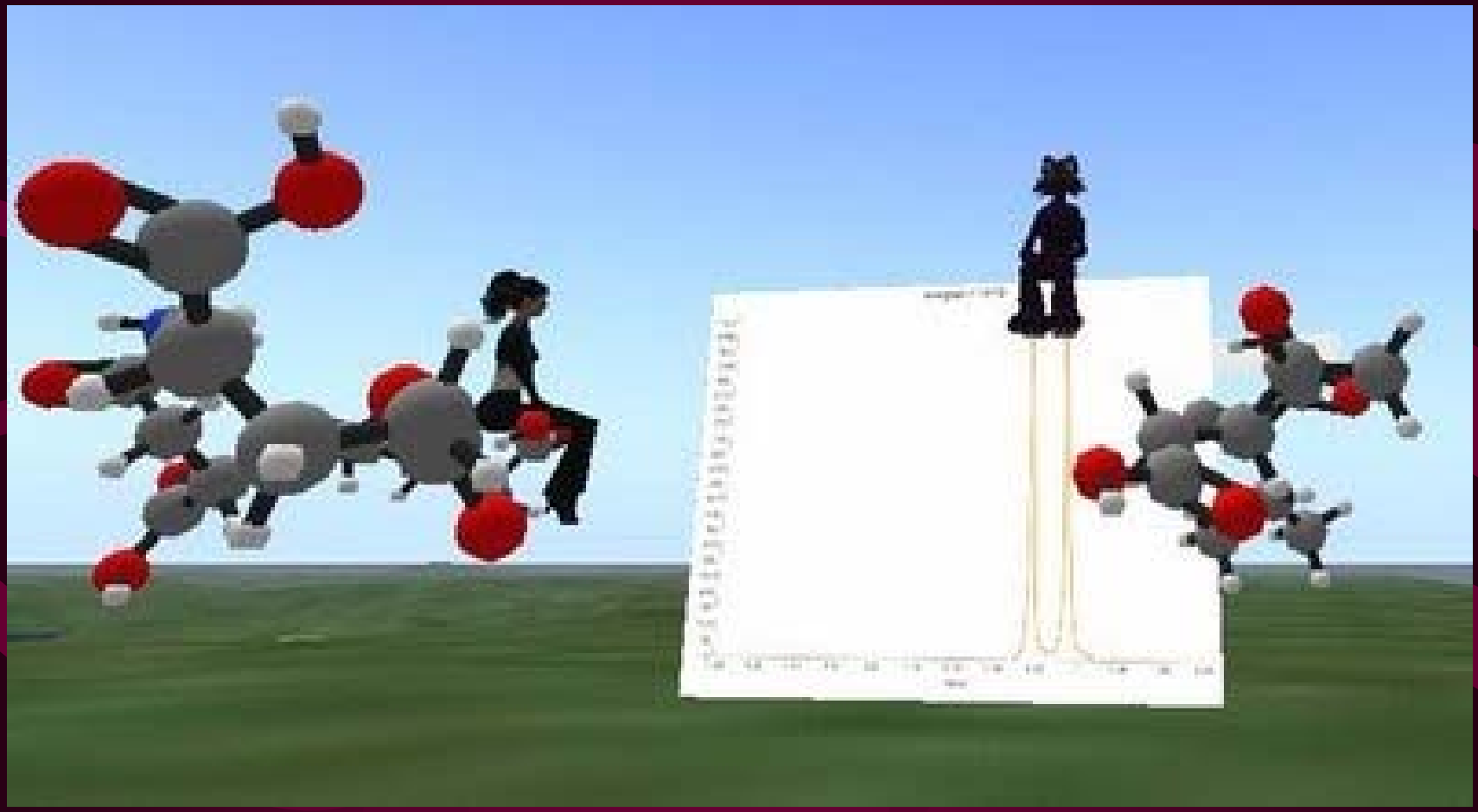
Remove Flags and Comments

Over 100,000 spectrum views so far - worldwide

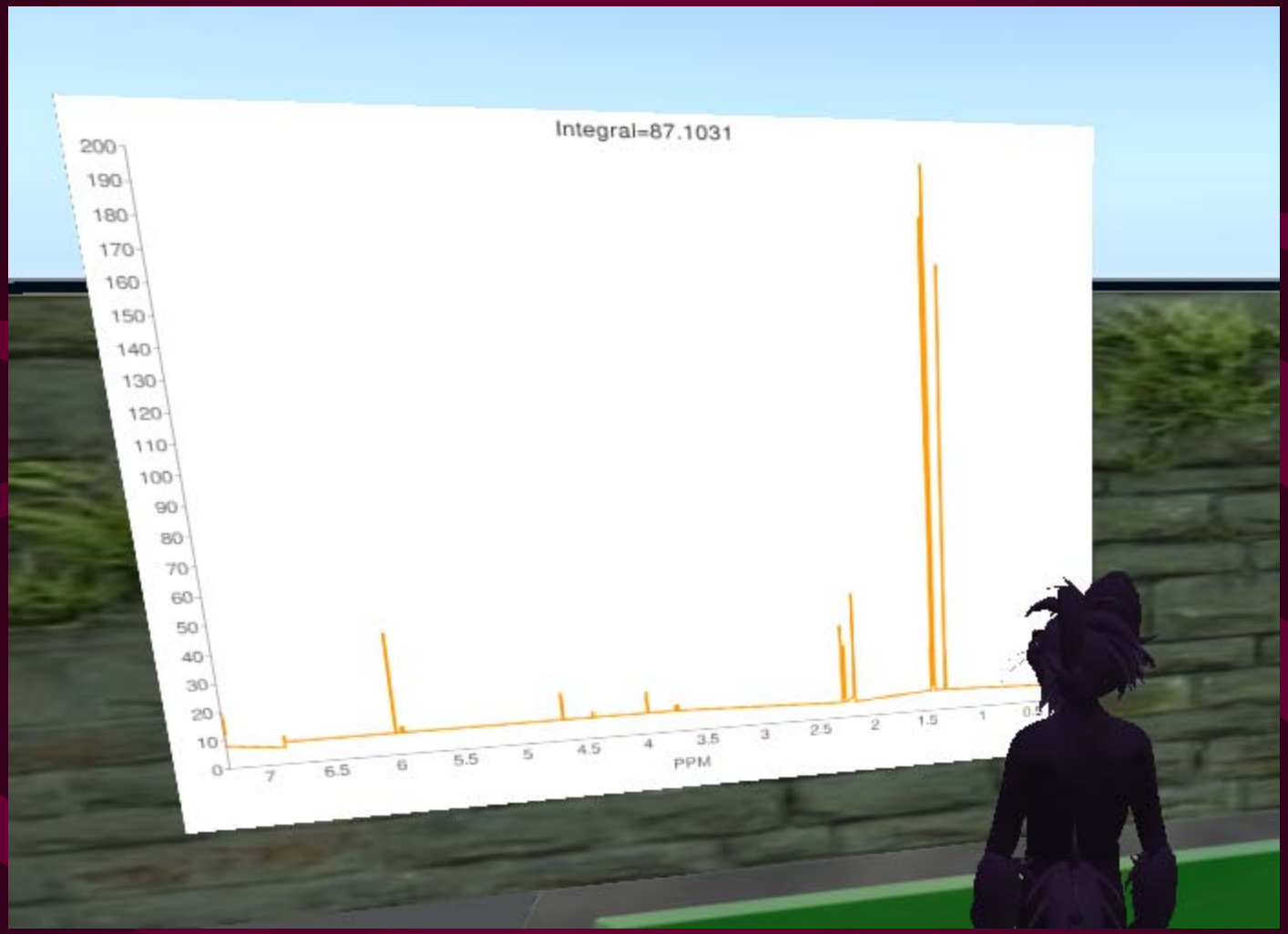
Top Scores

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

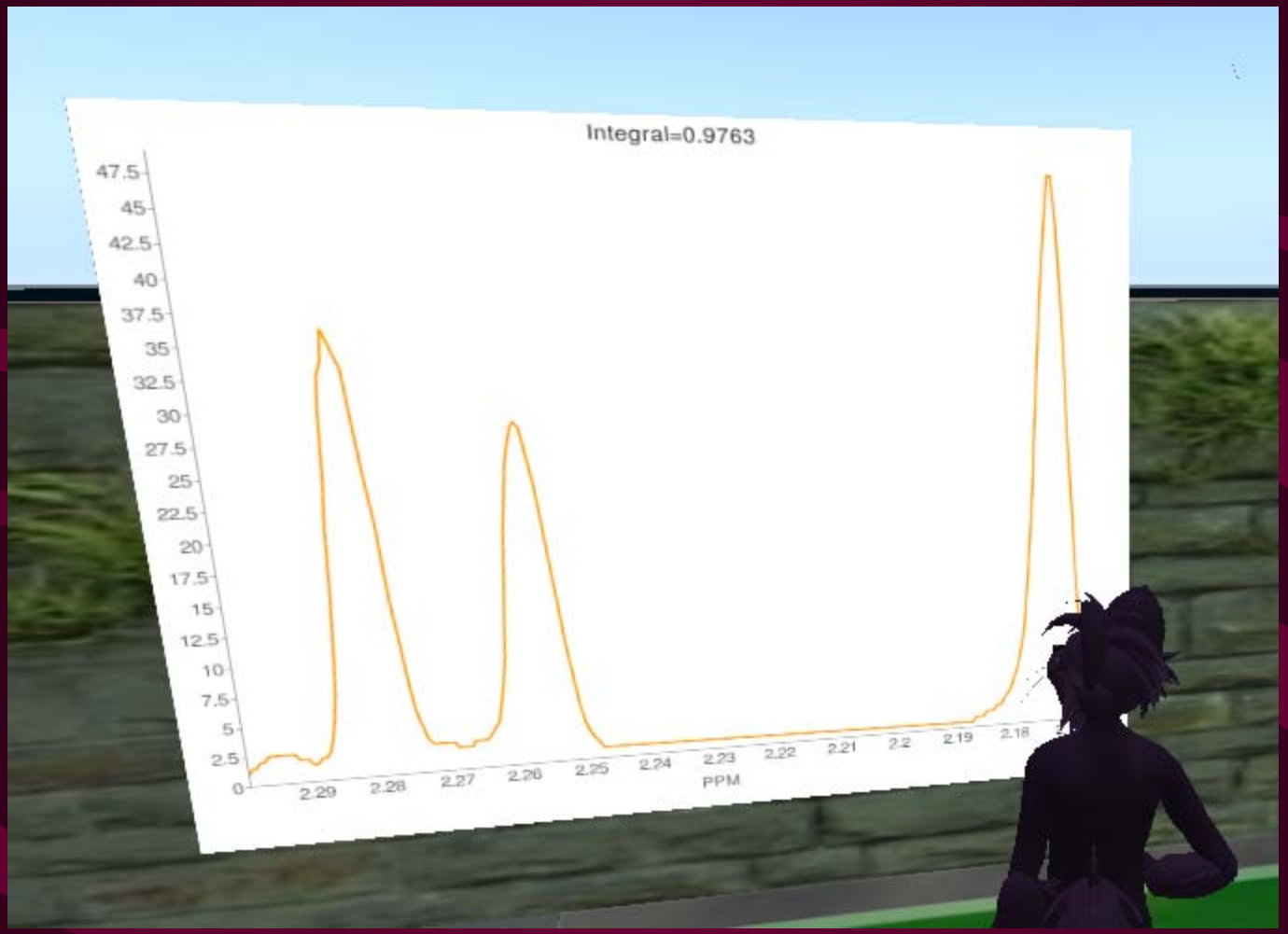
Spectral Game in Second Life (Andy Lang)



Interacting with the spectra via chat



Say: zoom 2.1-2.3



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)

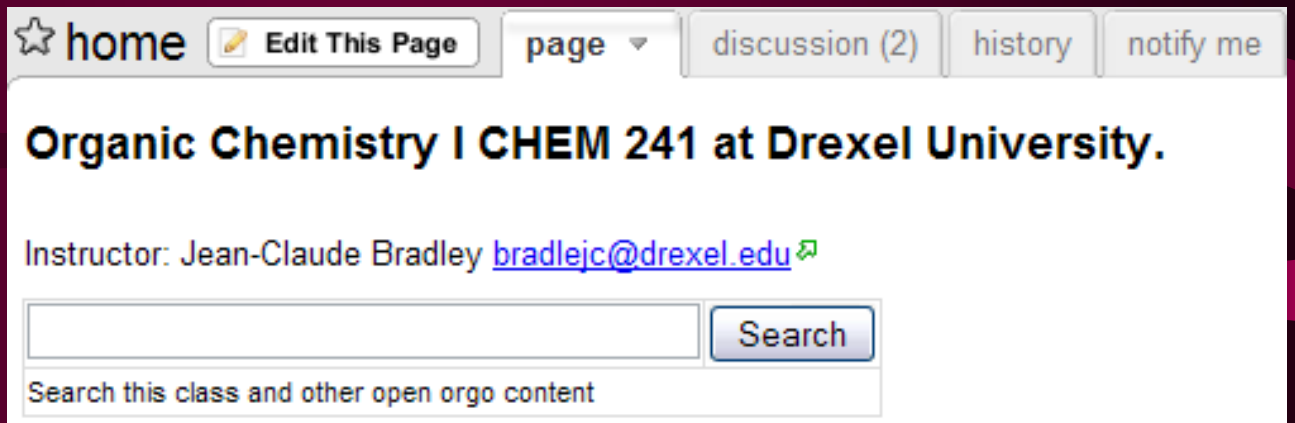
The following taken from Organic Chemistry II at Drexel University taught by Jean-Claude Bradley:

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

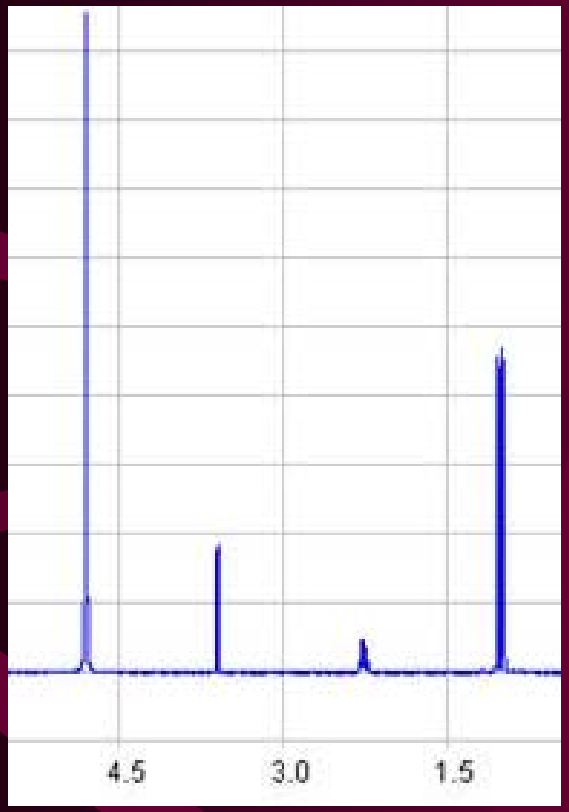
http://spectralgame.wikispaces.com/

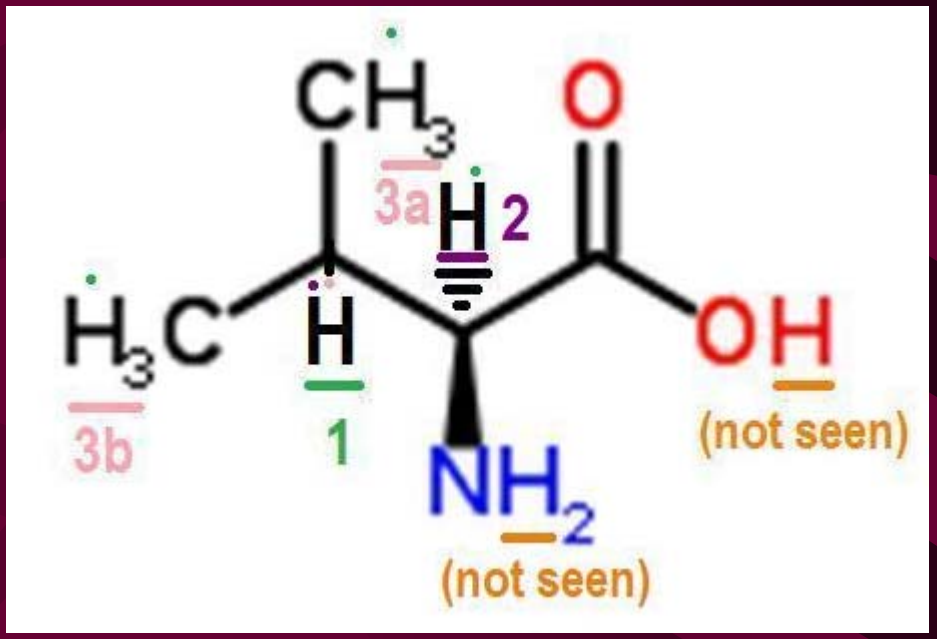
Class wiki



1. Content
2. Syllabus
3. FAQ
4. Archived Lectures on Class Blog (access or download files one by one)
5. Archived Lectures as ZIP files (download all M4V, MP3 and PDFs at once)
6. Lecture Transcript (ignore any information about specific dates or make-up policy)
7. Quizzes and tests are accessed via one.drexel.edu (demo account use chemguest, password education http://learning.dcollege.net)
8. Extra Credit Option
9. Taking quizzes on the ChemTile Game (First prize - top Drexel ALL score on Wednesday May 27, 2009 9:50AM)
10. First 4 chapters of Wade Organic Chemistry Edition 5 (problem set included)
11. Other textbooks and resources
12. Test Info
13. Assigned Problems (Eds 5 and 6 have same numbers)
14. Problem Solutions (downloadable m4v video files)

Neeraj's Analysis of the H NMR of valine on ChemSpider (wiki based assignment)

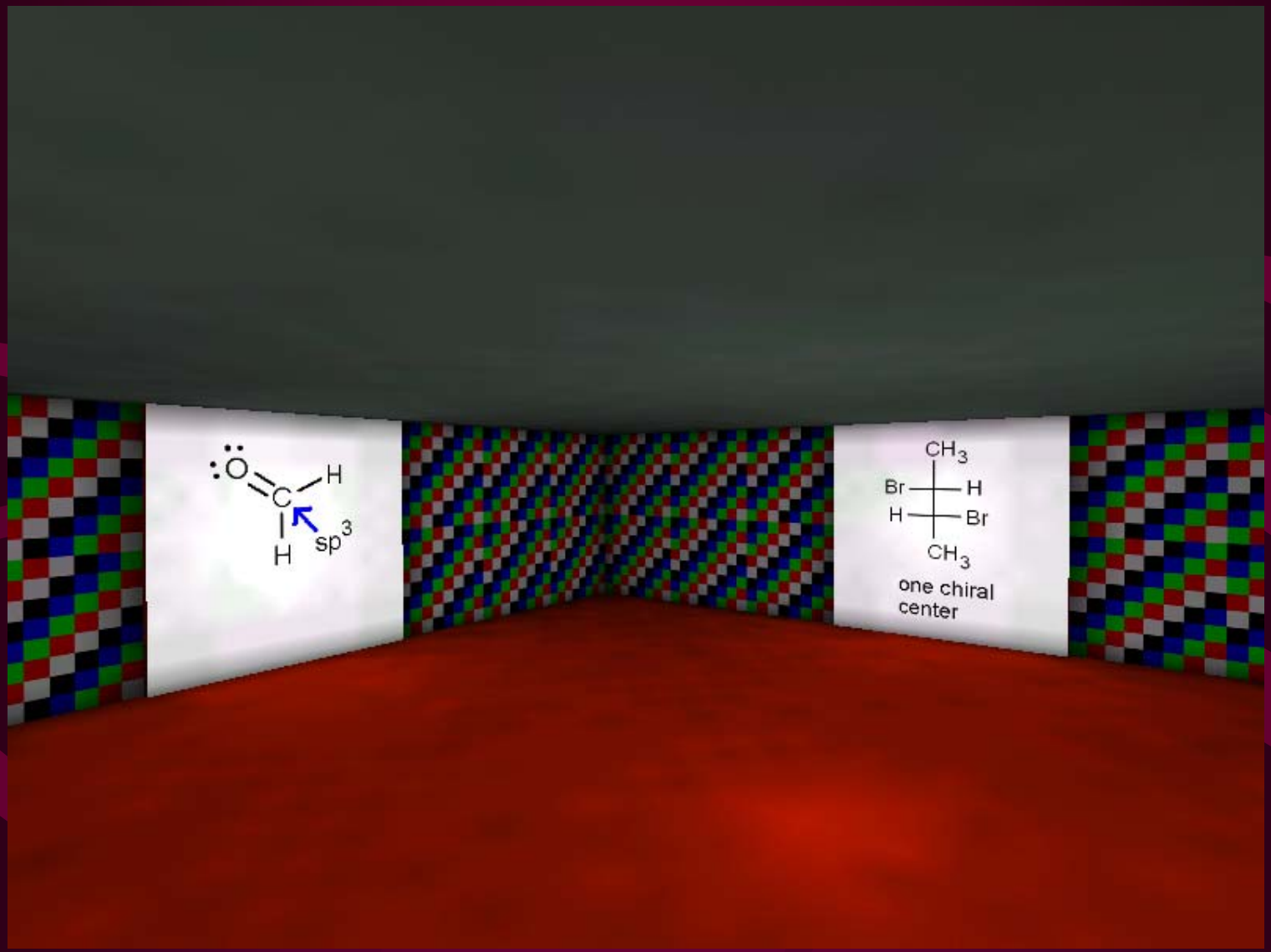




The two Hydrogens on the Amine group do not form peaks on the spectrum because they are exchanged in the solvent.

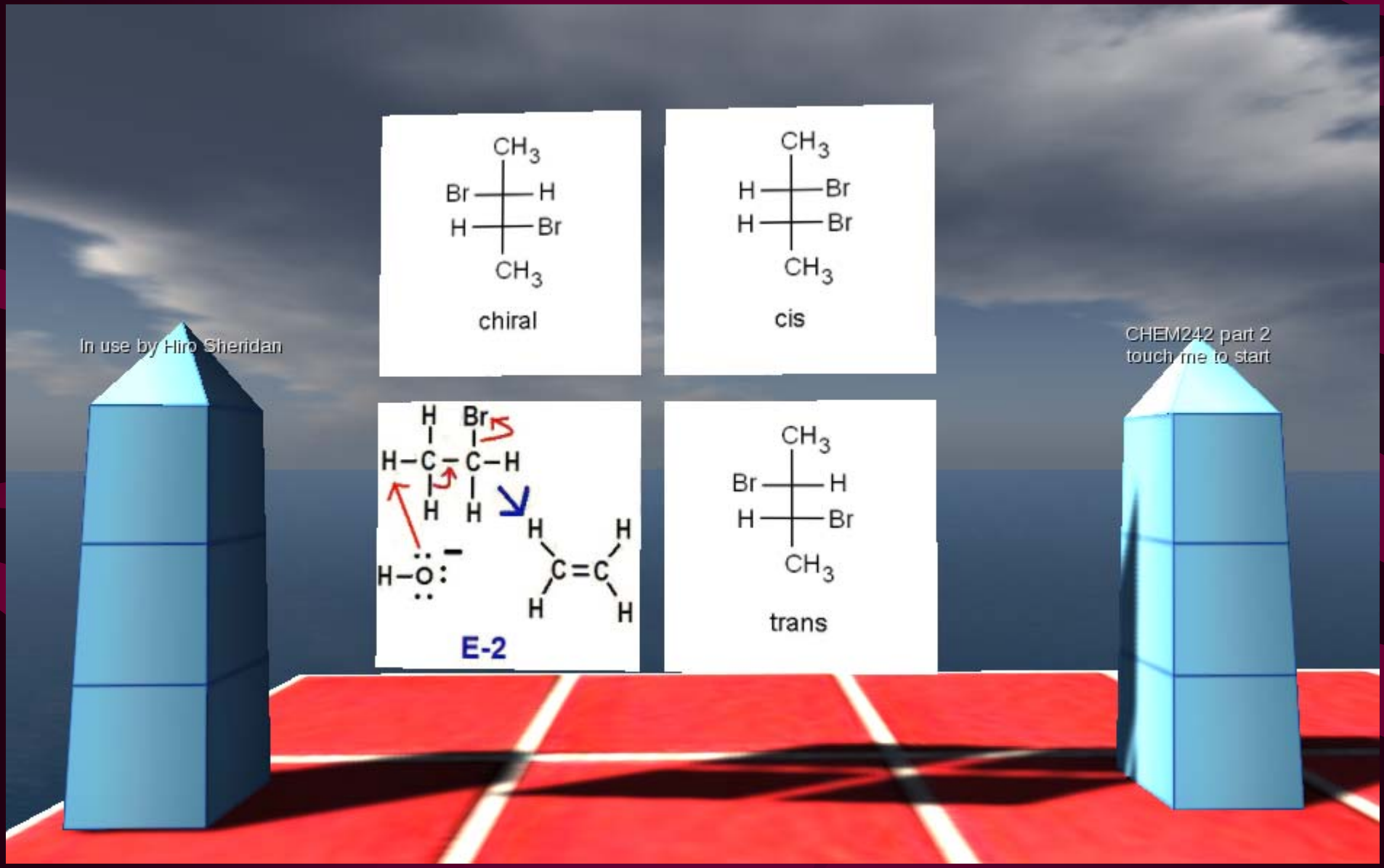
http://chem242.wikispaces.com/extracredit

EduFrag Maze (without weapons)

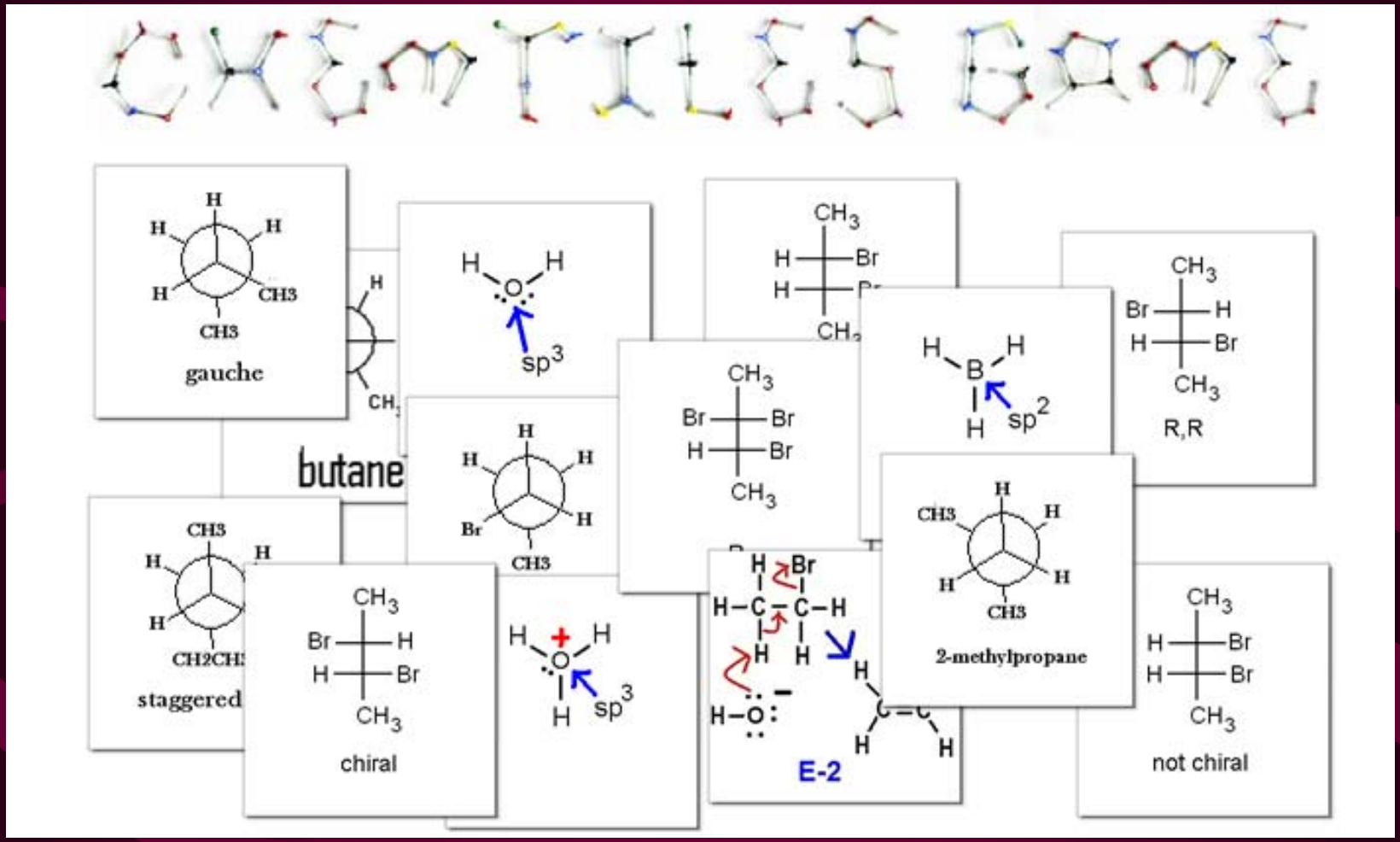


EduFrag Unreal Tournament (with weapons)

Quiz Obelisks in Second Life (Eloise Pasteur)



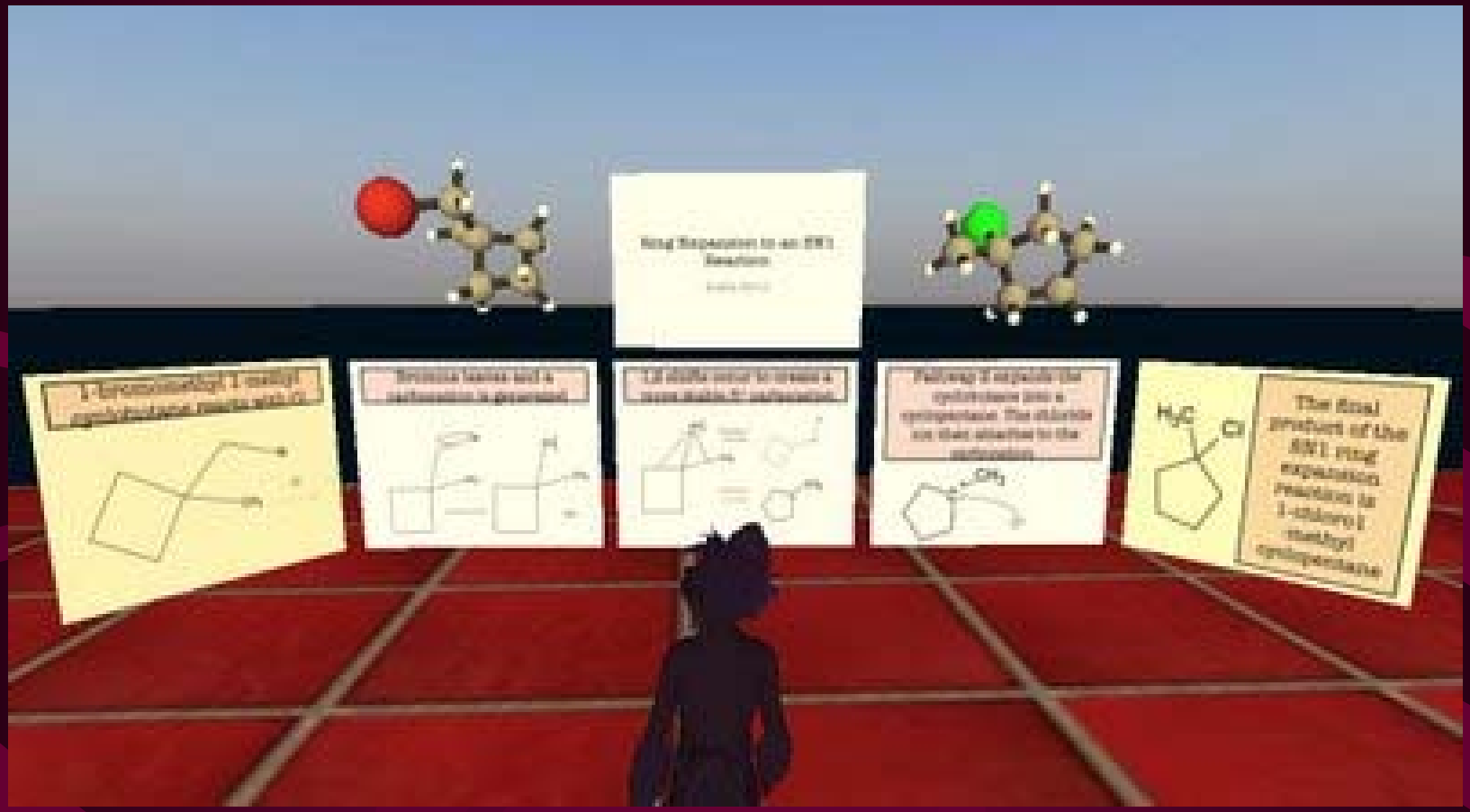
Remixing Code and Content (Andy Lang)



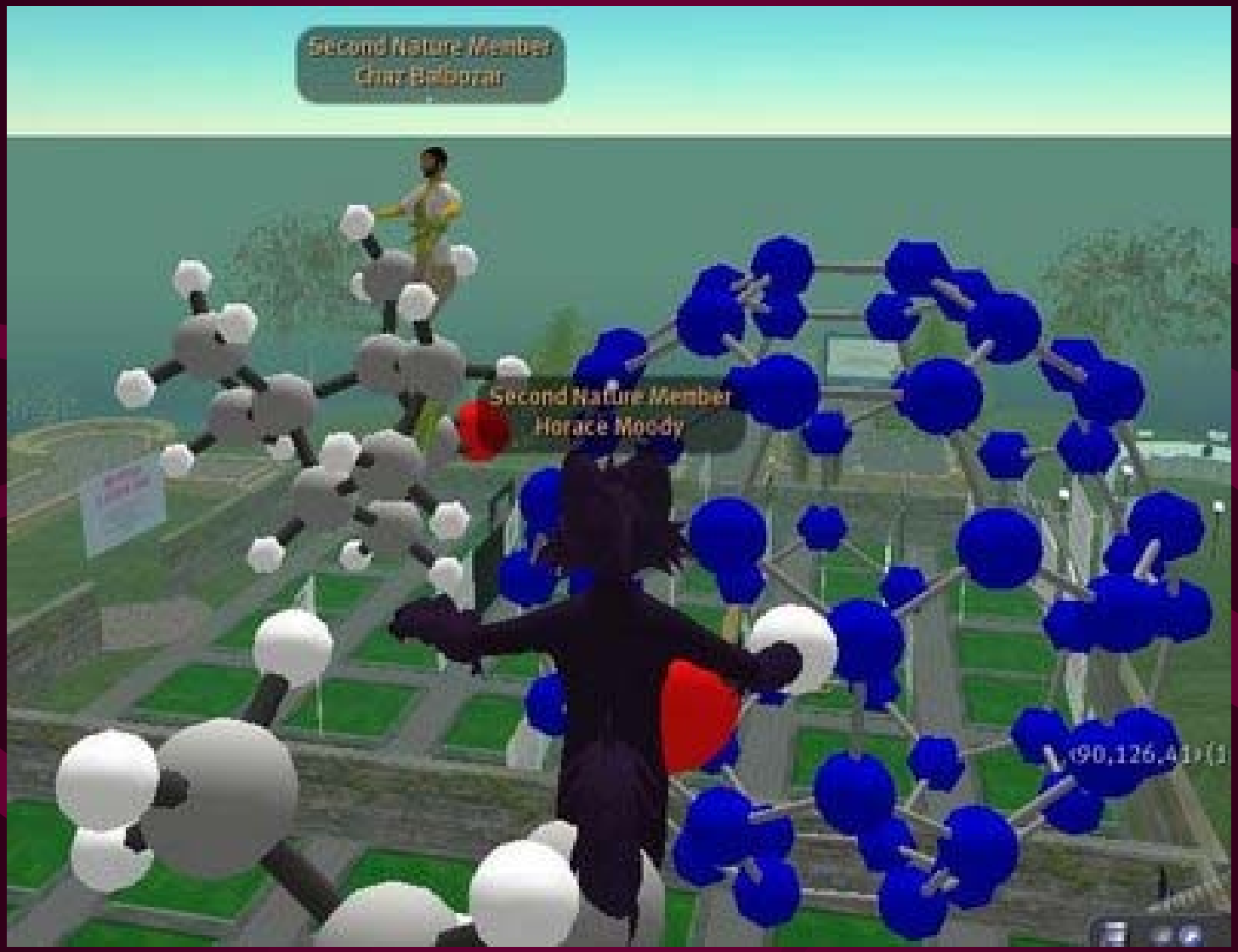
http://chem241.wikispaces.com/

Student Assignments in Second Life

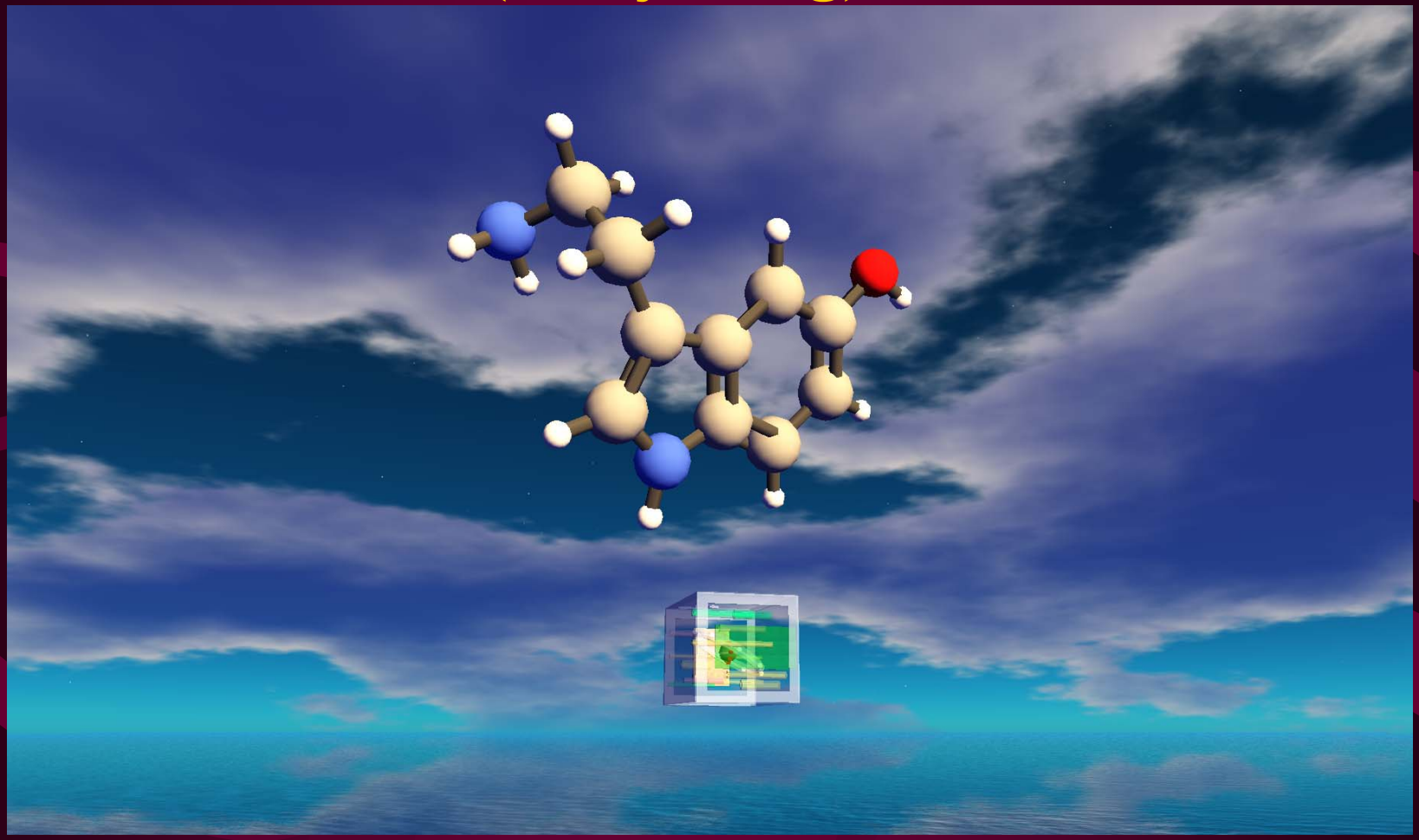
Student Created Exhibits on ACS Island



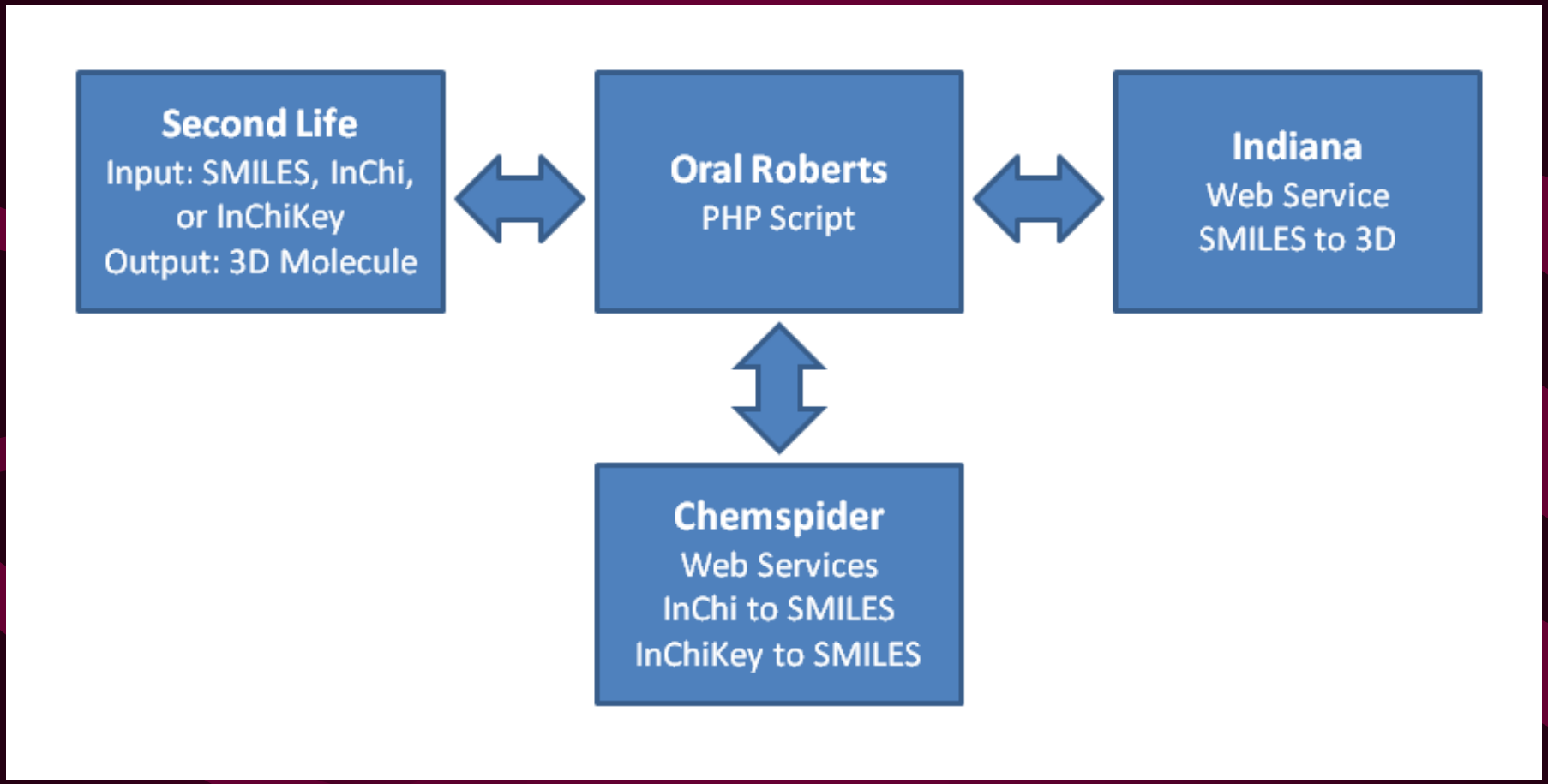
Flying Around on a Molecule



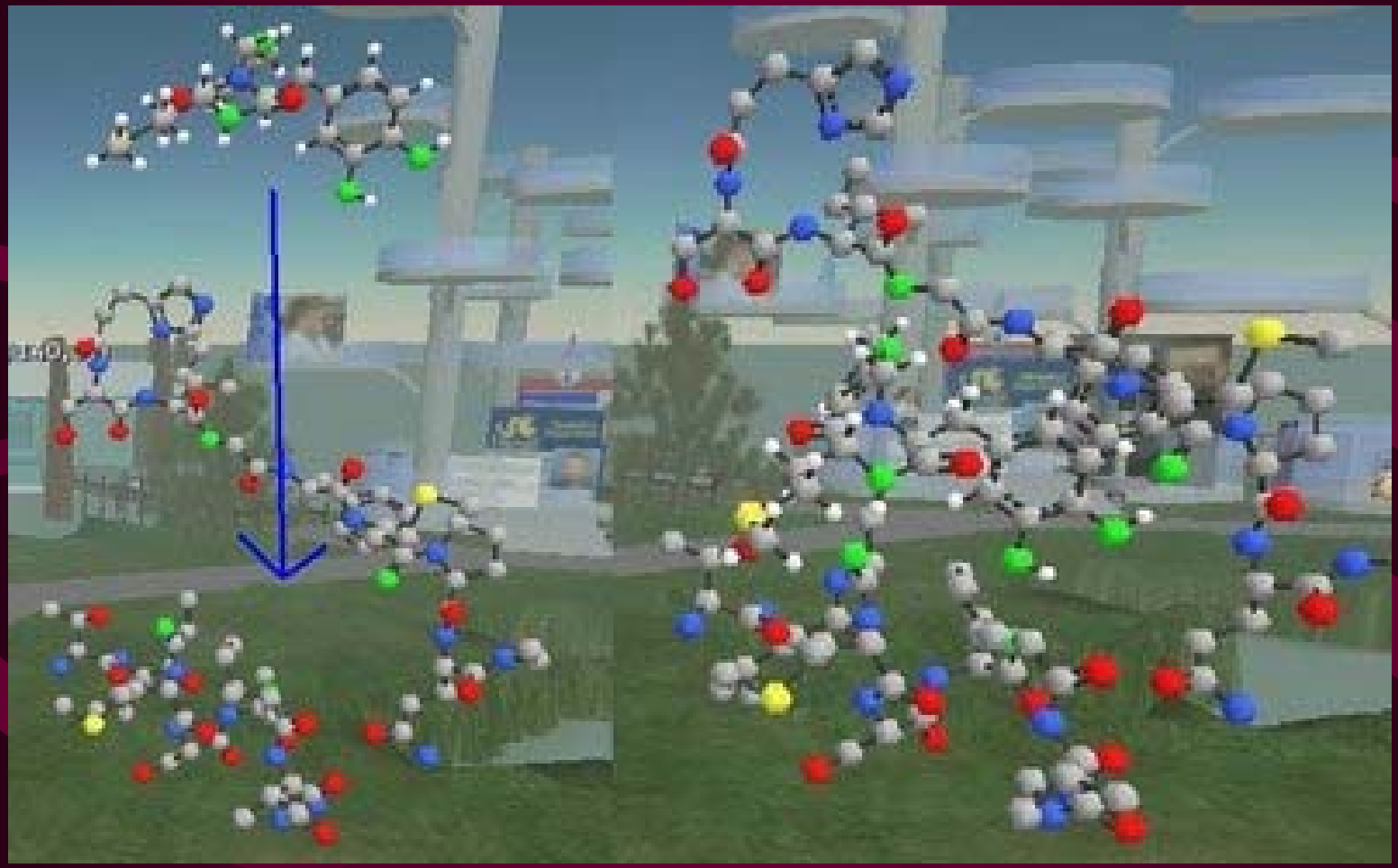
Orac: The 3D Molecule Rezzer
From SMILES, InChIs and InChIKeys to 3D Structure
(Andy Lang)



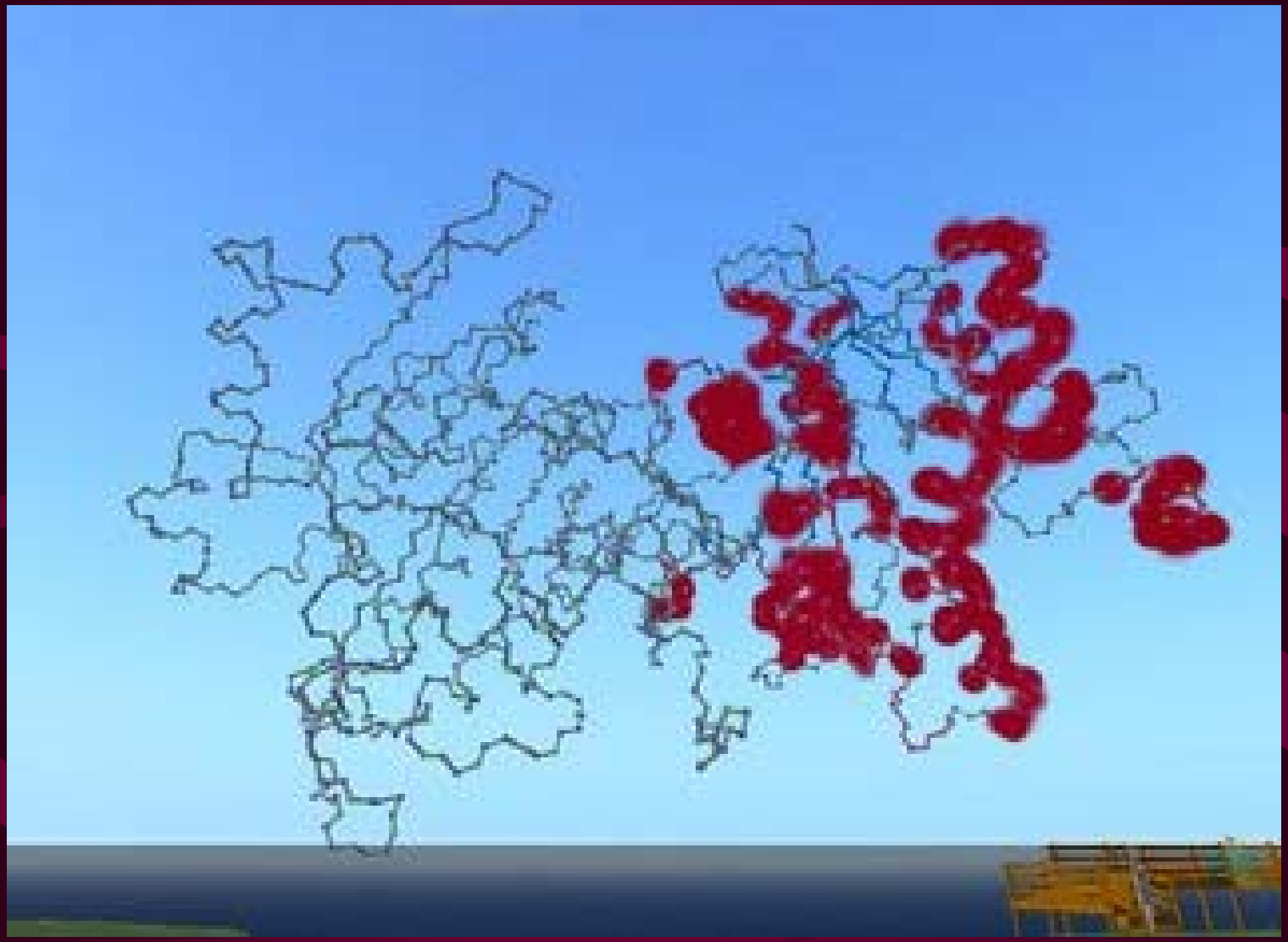
How Orac Works



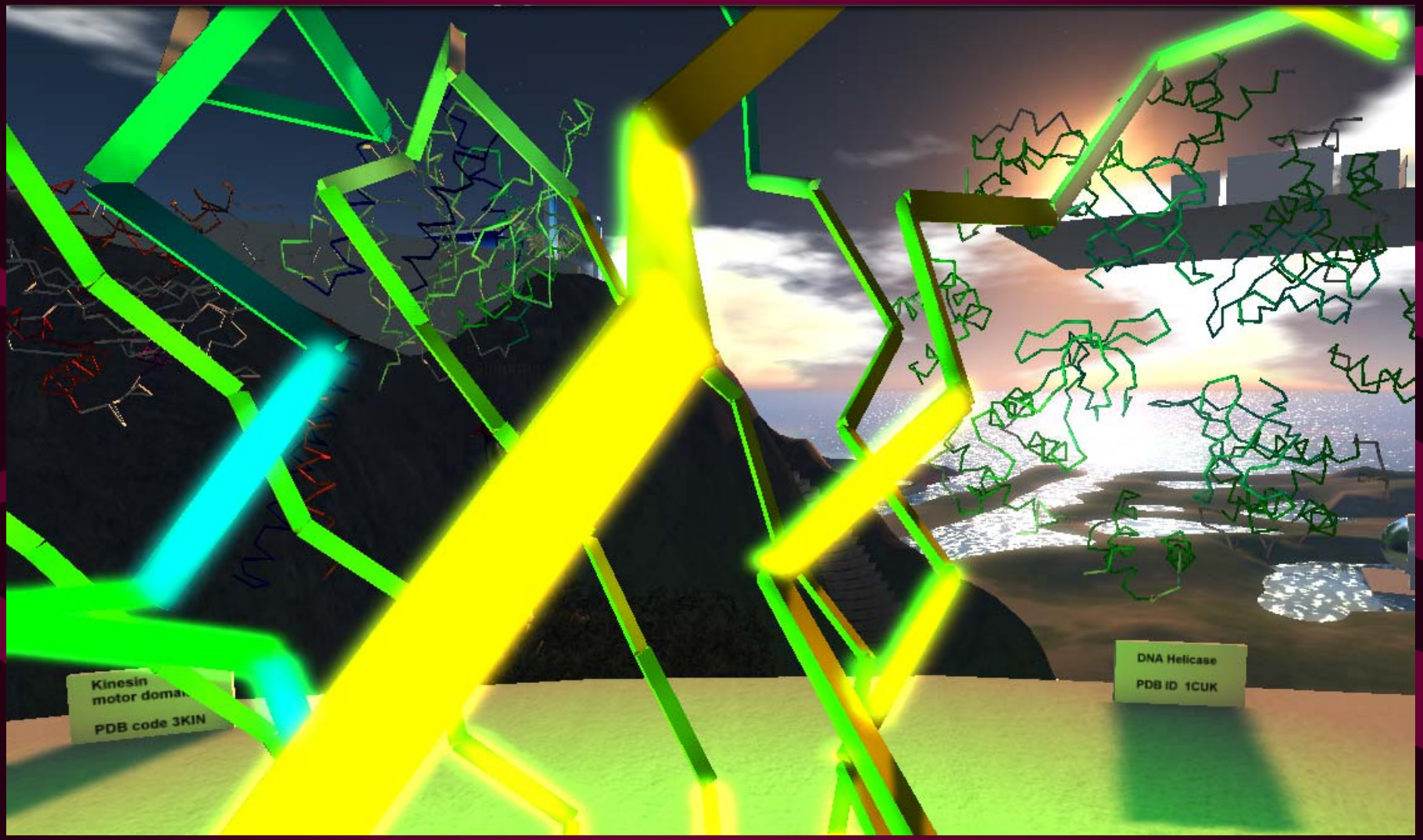
Docking Demonstration on Drexel Island



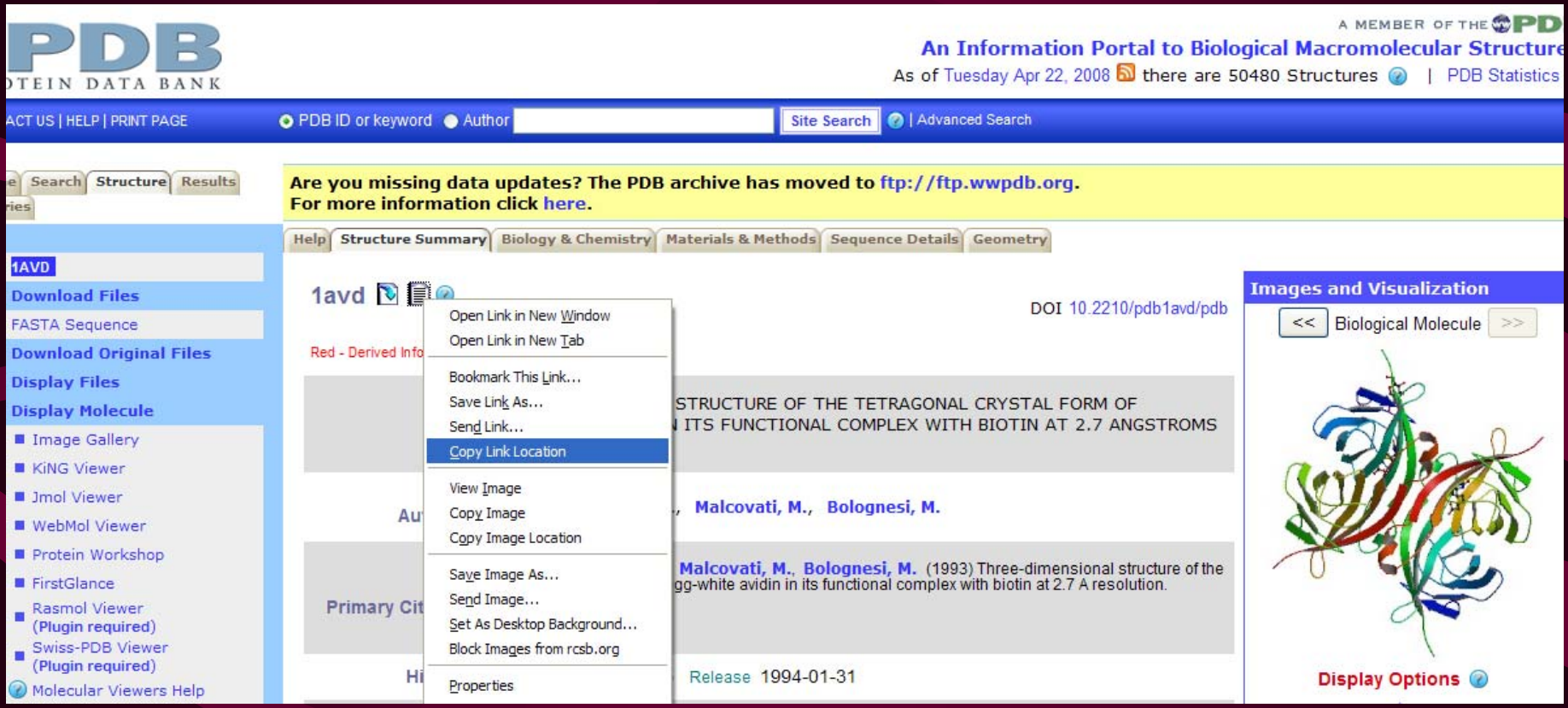
Enoyl Reductase (Peter Miller)



Green Fluorescent Protein (David Reeves)

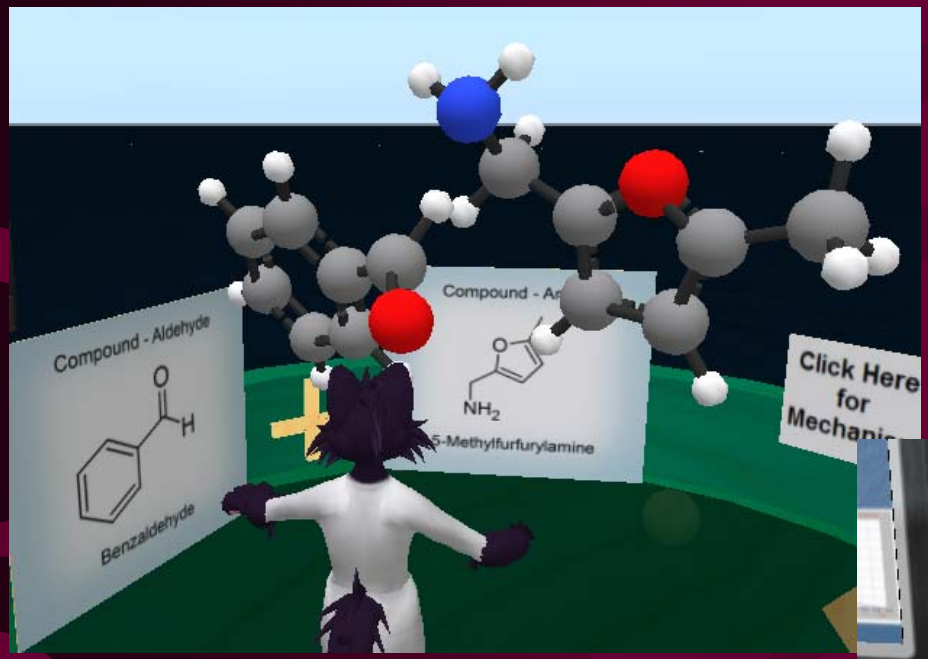


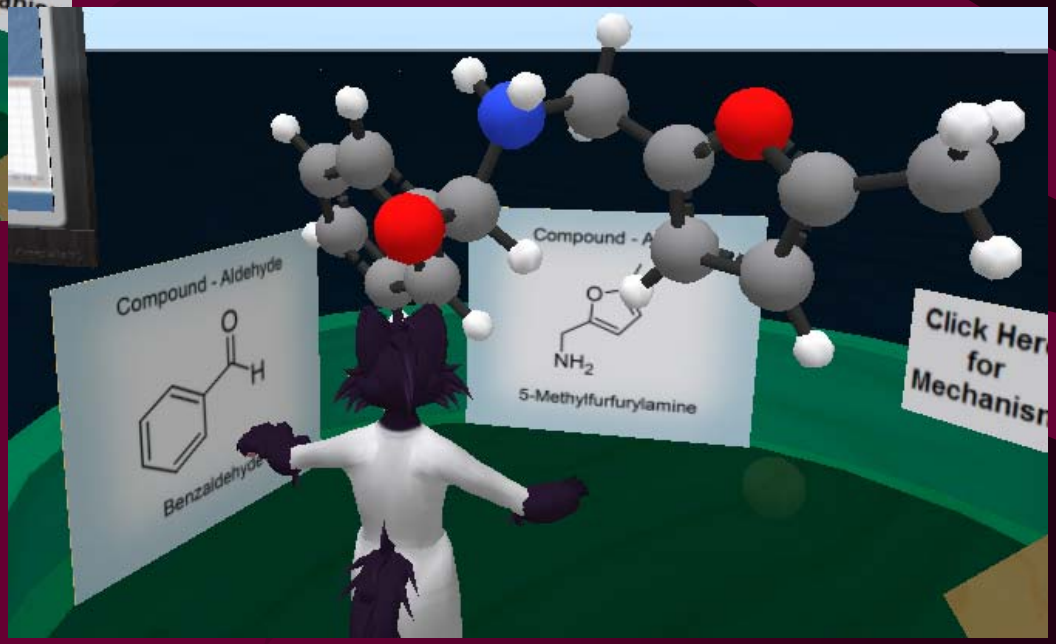
Avidin: From PDB file to…..



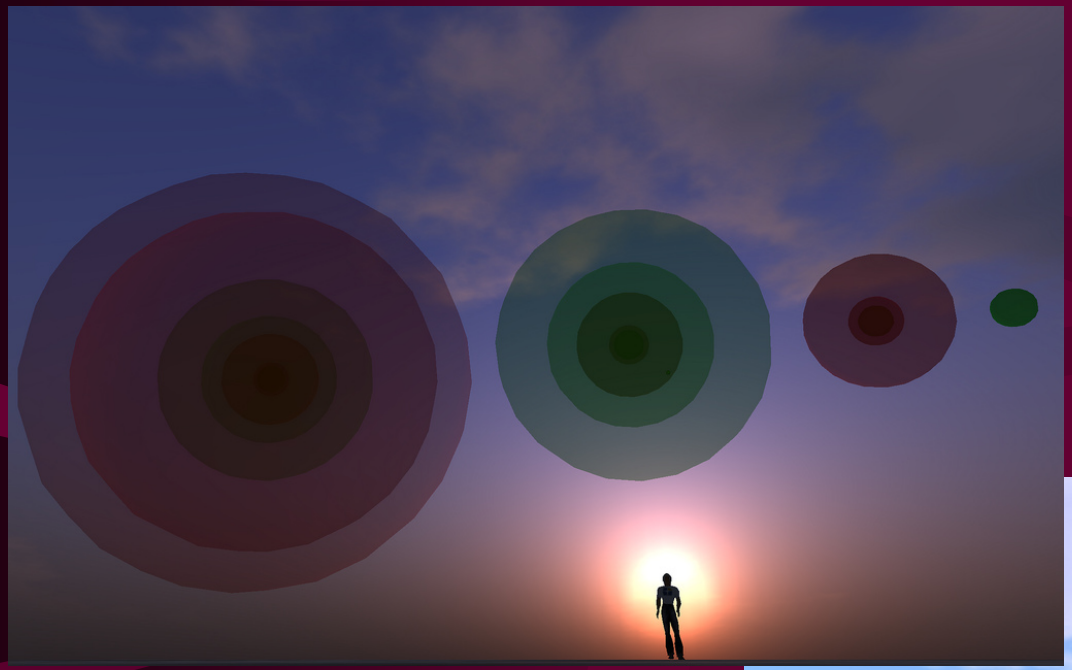
Avidin 3D structure in Second Life

Imine Formation Mechanism: Talk to the molecules!

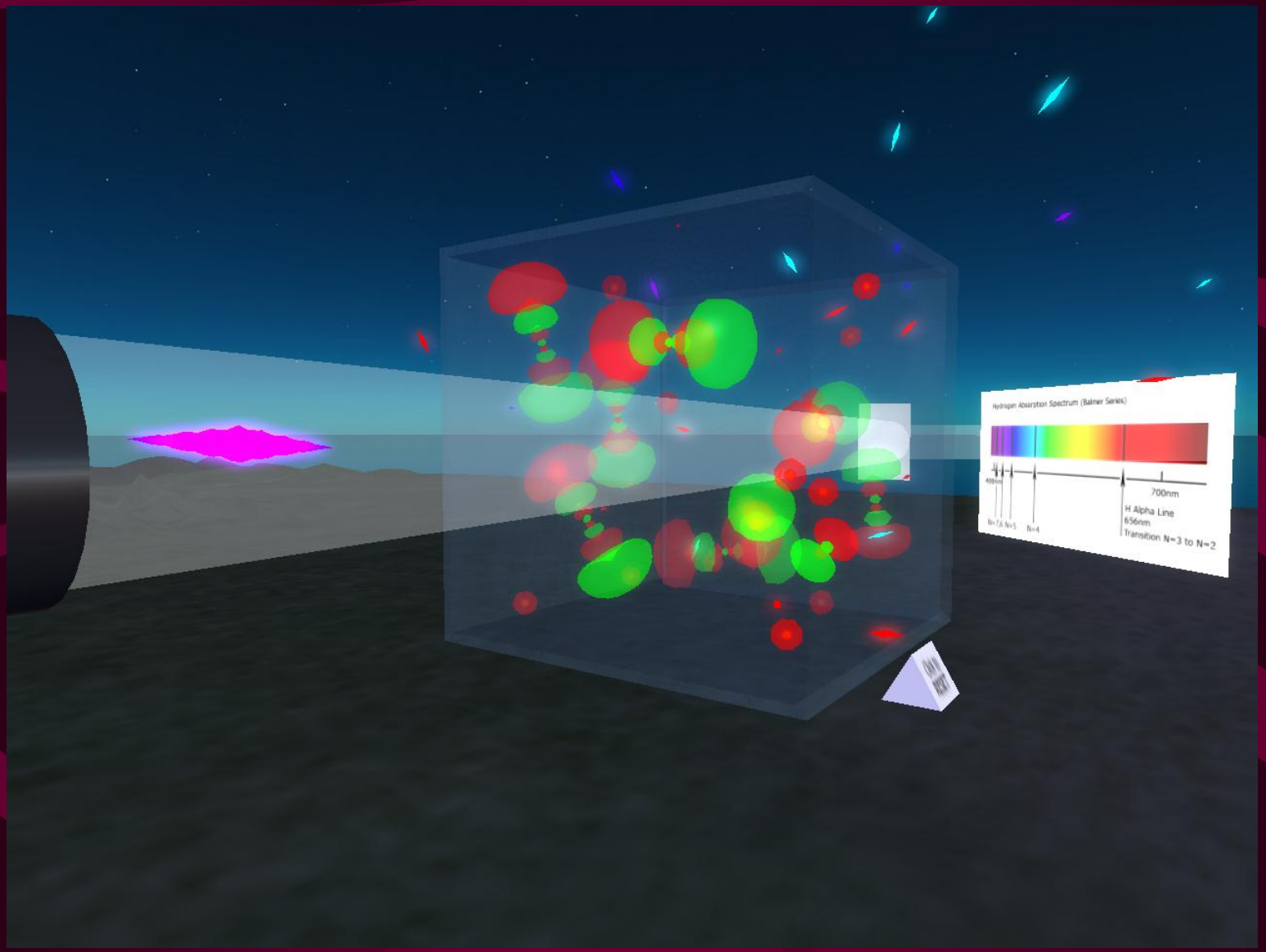




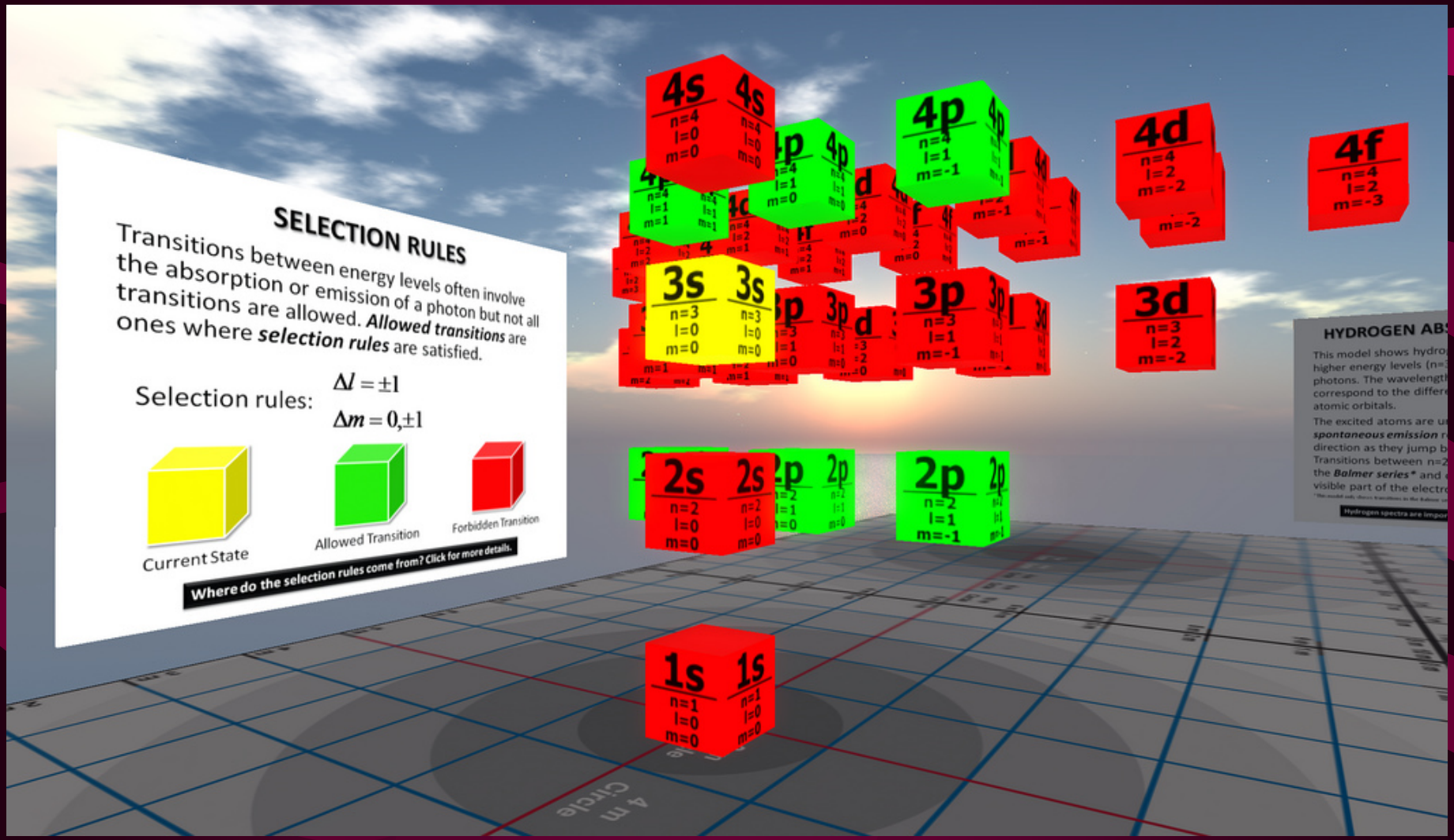
Atomic Orbitals



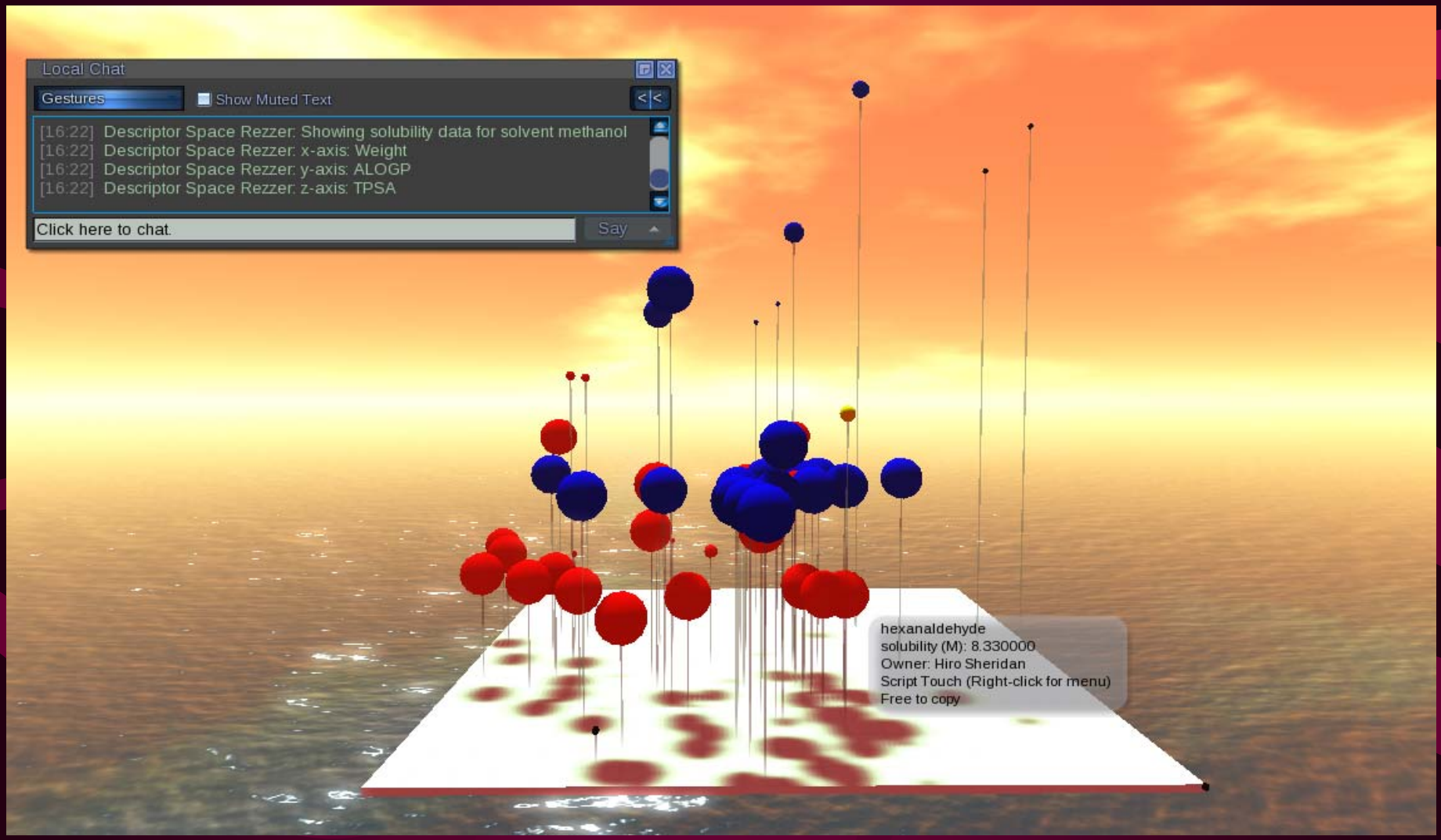
Hydrogen Absorption Spectrum



Selection Rules



5D Solubility Data Chemical Space



3D Periodic Table (ACS Freebie)

Faculty “Offices” on Drexel Island

Bradley Lab on Drexel Island

Posters on Second Nature – with Bells

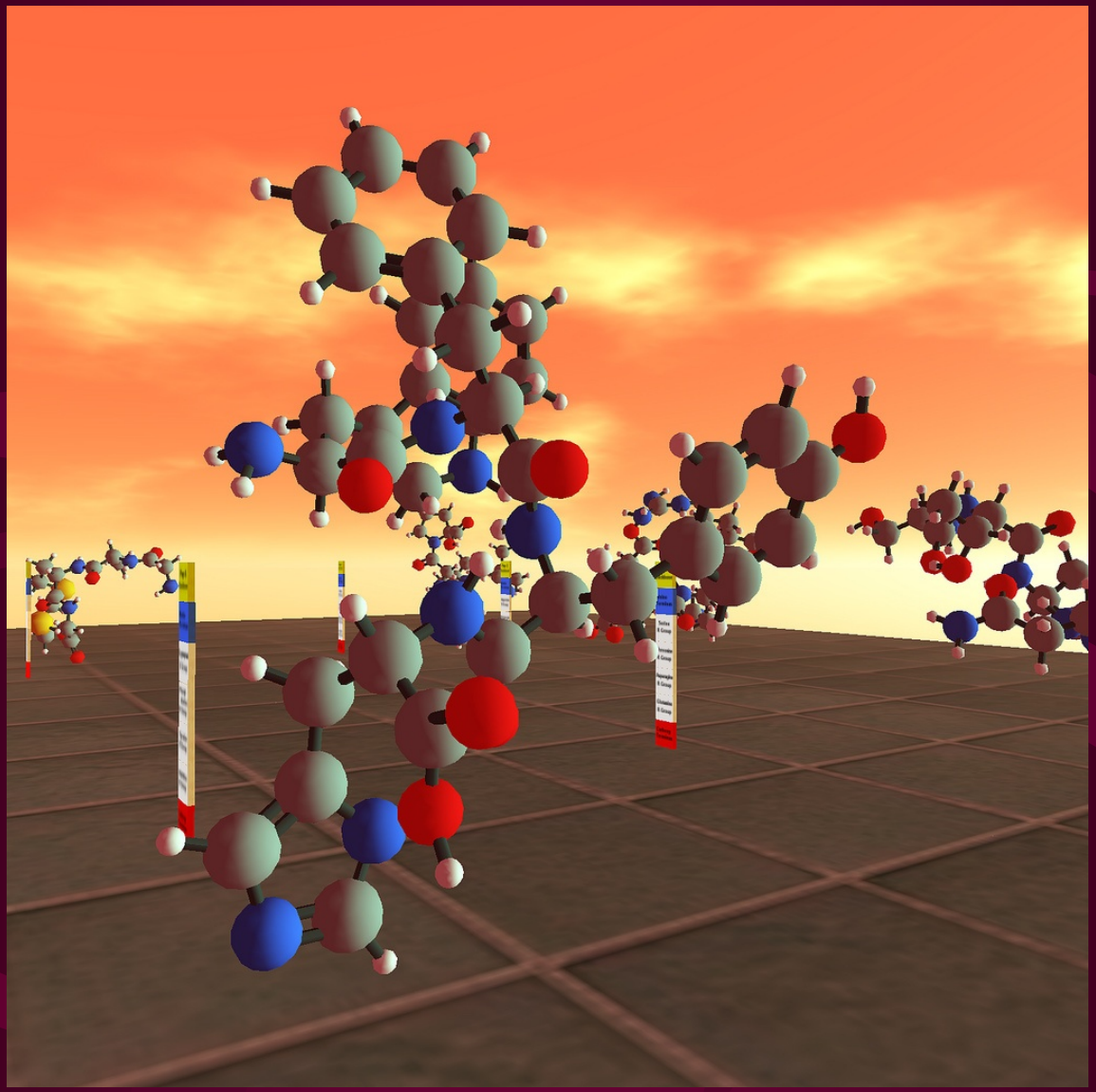
Conferences on Second Nature

Virtual Poster Area on ACS island

Resident Chemist Program: Hinestroza Lab

Virtual Lab (Kurt Winkelmann)

Amino World (Joan Slonczewski)

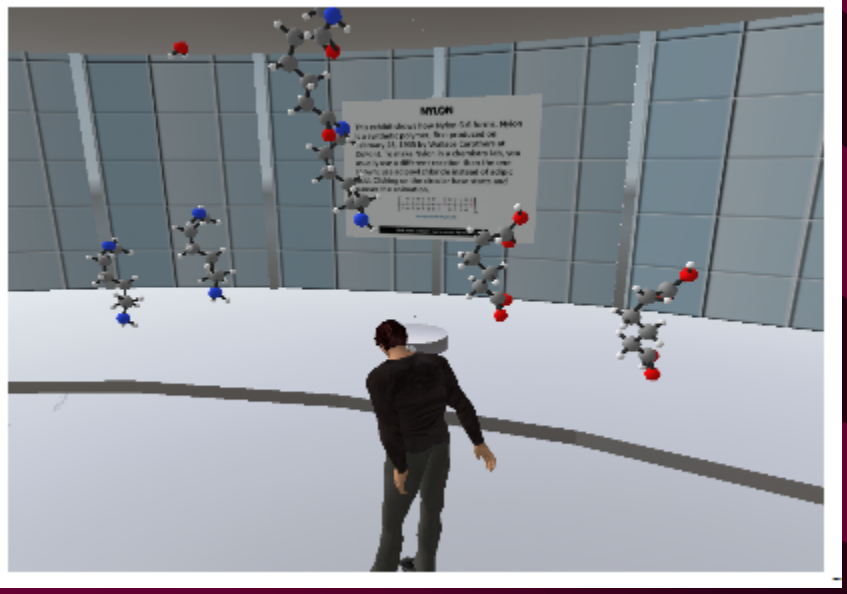


Student assignment: networking in Second Life and FriendFeed

Second Life Interviews (Second Life Names)

Arij Pevensey is a student (majoring in chemistry for three years now) who is i
molecules.
Georgianna Blackburn is an e-marketer (for Sigma Aldrich for two
delivery and joined Second Life in order to investigate new technolo
Hiro Sheridan is a professor (of mathematics @ ORU and has bee
and multi-dimensional chemical data visualization and joined Secon
chemical data visualizations in Second Life).

Nylon polymerization (http://slurl.com/secondlife/ACS/176/239/25)



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Chemistry Central Journal

http://www.journal.chemistrycentral.com/content/3/1/1

4 Accesses 4893

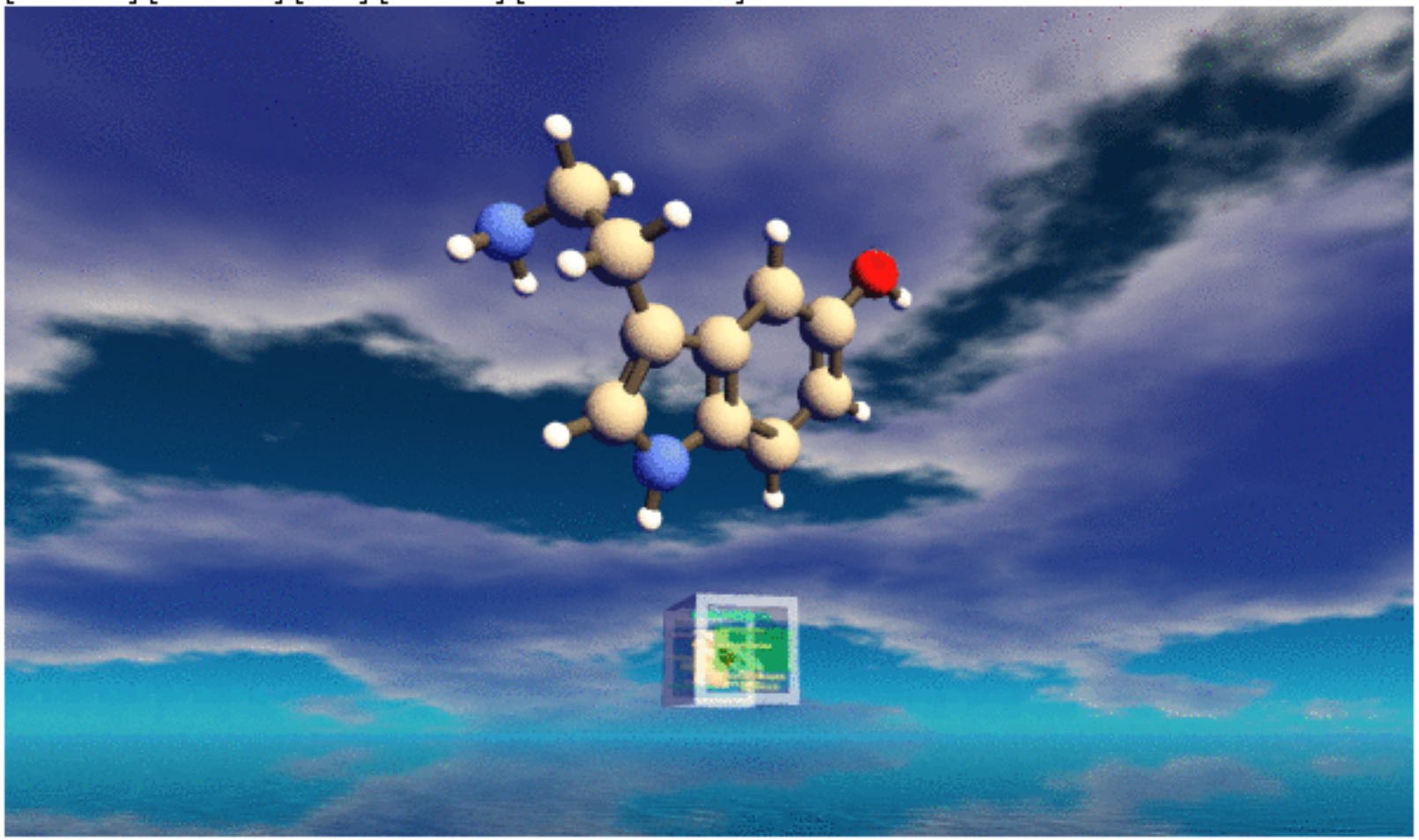
4. Review Open Access Highly accessed

Chemistry in Second Life

Andrew SID Lang, Jean-Claude Bradley

Chemistry Central Journal 2009, **3**:14 (23 October 2009)

[Abstract] [Full Text] [PDF] [PubMed] [Related articles]



Conclusions

- Think about your educational objectives
- Experiment with technology
- Keep what works
- To make this efficient learn from others