Open Notebook Science: Does Transparency Work?

HUBzero Conference

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April 6, 2011

The current state of transparency in scientific communication

Case study of melting point data

The Chemical Information Validation Sheet

567 curated and referenced measurements from
Fall 2010 Chemical Information Retrieval course

	CSID	data source	data source type	experimental or predicted	property	source value	source units	common value	common units	link
DDT	2928	MSDS	database - government	experimental	boiling point	260	C	260	C	http://msds.chem.ox.ac.uk/
DDT	2928	CDC	database - government	experimental	boiling point	230	F	110	C	http://www.cdc.gov/niosh/np
DDT	2928	Wikipedia	website - commercial	experimental	boiling point	260	C	260	C	http://en.wikipedia.org/wiki/D
DDT	2928	HBCP	website - commercial	experimental	boiling point	260	C	260	C	http://www.hbcpnetbase.con id=03_01_91&DocId=11738(
DDT	2928	Chemspider	website - commercial	predicted	boiling point	416.2	C	416.2	C	http://www.chemspider.com Structure.2928.html

cheminfo2010.wikispaces.com

http://usefulchem.blogspot.com/2011/01/chemical-information-validation-results.html

The Chemical Information Validation Explorer

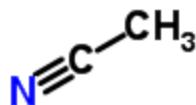onswebservices.wikispaces.com/ChemInfoValidation (Andrew Lang)

Discovering outliers for melting points (stdev/average)
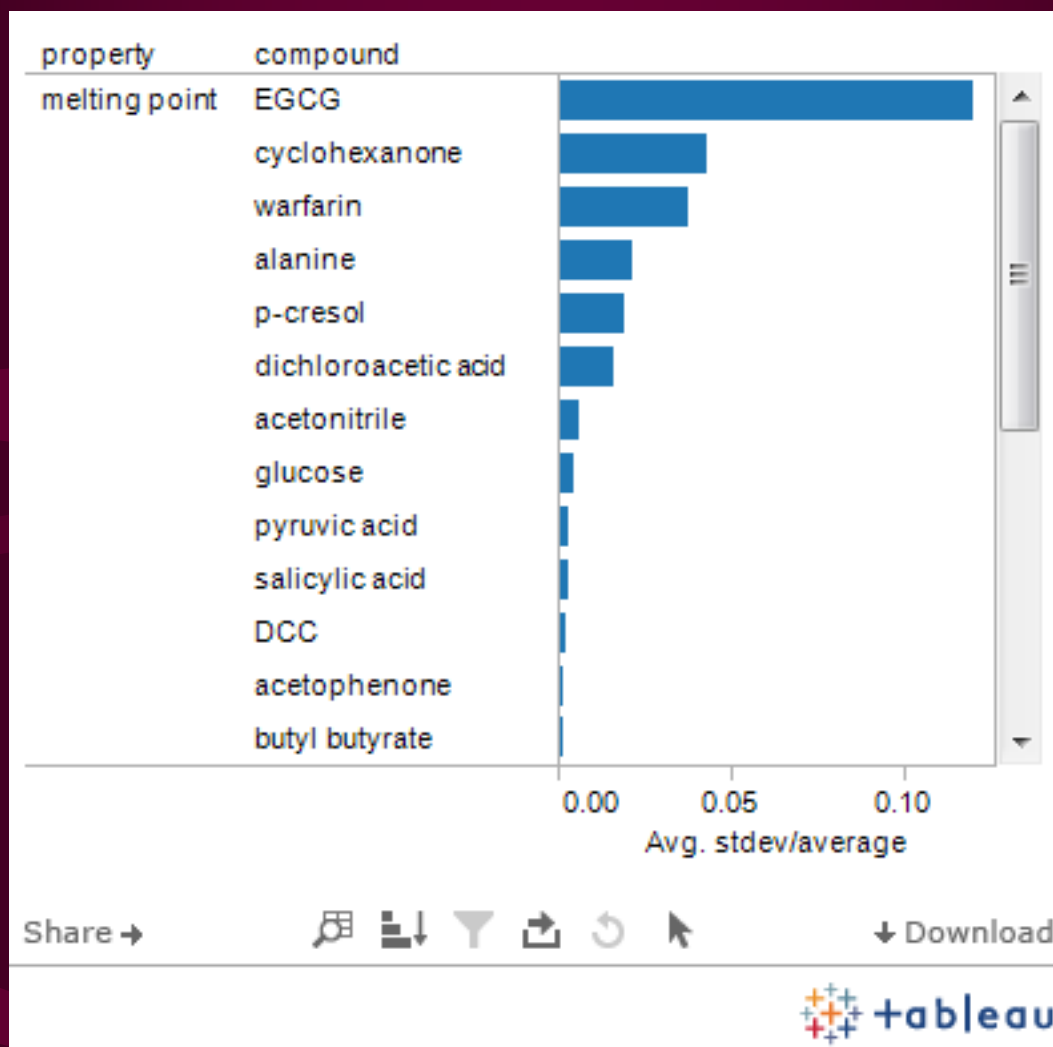
Investigating the m.p. inconsistencies of EGCG

Chemical Information Retrieval
Drexel University Course CHEM 367-767

Property Explorer

Common Name EGCG

Property melting point

EGCG
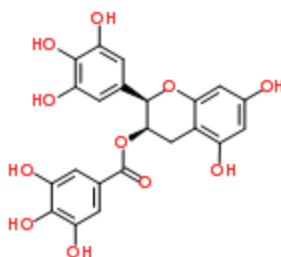
Statistics

Number of Results: 2

Average Value: 452.650 K

95% Confidence Interval: (399.292,506.008)

Standard Deviation: 38.500

Coefficient of Variation: 0.085

Value (K)	Source	Image	Credit	Source Type	Value Type	Notes
414.150	Chemistry of Natural Compounds		Jose Rafael Quejada	peer reviewed journal	experimental	
491.150	Merck Index		Jose Rafael Quejada	commercial database	experimental	

(-)-Epigallocatechin-3-O-gallate, $C_{22}H_{18}O_{11}$, $[M]^+$ 458, mp 140-142°C.

CAS Name	synonyms	tradename(manufac	CAS Registry No.	mol. formula	mol. weight	melting point (°C)
3,4,5-Trihydroxybei	view synonyms		989-51-5	$C_{22}H_{18}O_{11}$	458.37	mp 218°

Investigating the m.p. inconsistencies of cyclohexanone

Property Explorer

Common Name [cyclohexanone ▼]

Property [melting point ▼]

cyclohexanone
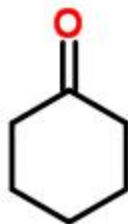
Statistics

Number of Results: 5

Average Value: 233.350 K

95% Confidence Interval: (225.444,241.256)

Standard Deviation: 9.020

Coefficient of Variation: 0.039

Value (K)	Source	Image	Credit	Source Type	Value Type	Notes
226.150	Acros		Byron Forte	chemical vendor	experimental	
247.150	Alfa Aesar		Byron Forte	chemical vendor	experimental	
241.150	Oxford		Byron Forte	academic website	experimental	
226.150	Sigma-Aldrich		Byron Forte	chemical vendor	experimental	
226.150	Wolfram Alpha		Byron Forte	free database	experimental	

Sigma-Aldrich, Acros and Wolfram Alpha apparently use the same sources for melting points

Sigma-Aldrich, Acros and Wolfram Alpha apparently use the same sources for boiling points

Sigma-Aldrich, Acros and Wolfram Alpha apparently DO NOT use the same sources for flash points

Most popular data sources
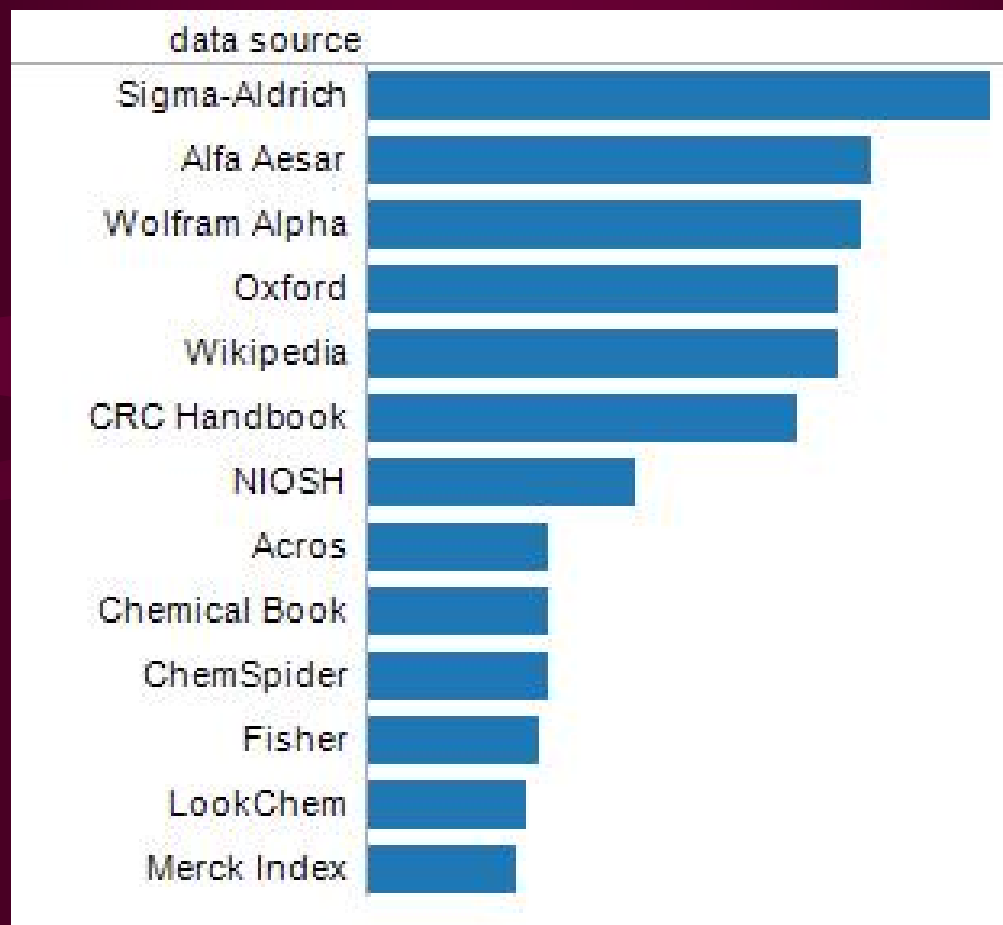
Alfa Aesar donates melting points to the public

DSSTK	DSDESC	DSPURE	DCMELT
H26903	(-)-1,4-Di-O-tosyl-2,3-O-isopropylidene-L-threitol	98%	90°
B24134	(-)-2,3-O-Isopropylidene-D-threitol	98%	45-49°
L04759	(-)-alpha-Pinene	98%, cont. variab	-64°
A12684	(-)-Borneol	98%	205-208°
A18040	(-)-Camphene	tech. 80%	ca 35°
A18796	(-)-Cinchonidine	99% (total base),	201-206°
A16180	(-)-Dibenzoyl-L-tartaric acid monohydrate	98+%	90-92°
A16181	(-)-Dibenzoyl-L-tartaric acid, anhydrous	99%	154-156°
A17992	(-)-Diethyl D-tartrate	99%	17°
B21029	(-)-DIOP	98%	88-90°
L15151	(-)-Fenchone	98+%	3-5°
L18485	(-)-Lupinine	97%	62-65°
41570	(-)-N-Methylephedrine	98+%	86°-88°
L04848	(-)-Shikimic acid	98%	184-188°
B23090	(+)-2,3-O-Isopropylidene-L-threitol	98%	45-49°
A11542	(+)-5-Iodo-2'-deoxyuridine	98%	ca 190° dec.

Open Melting Point Explorer

Outliers

MDPI dataset

EPI (via ChemSpider)
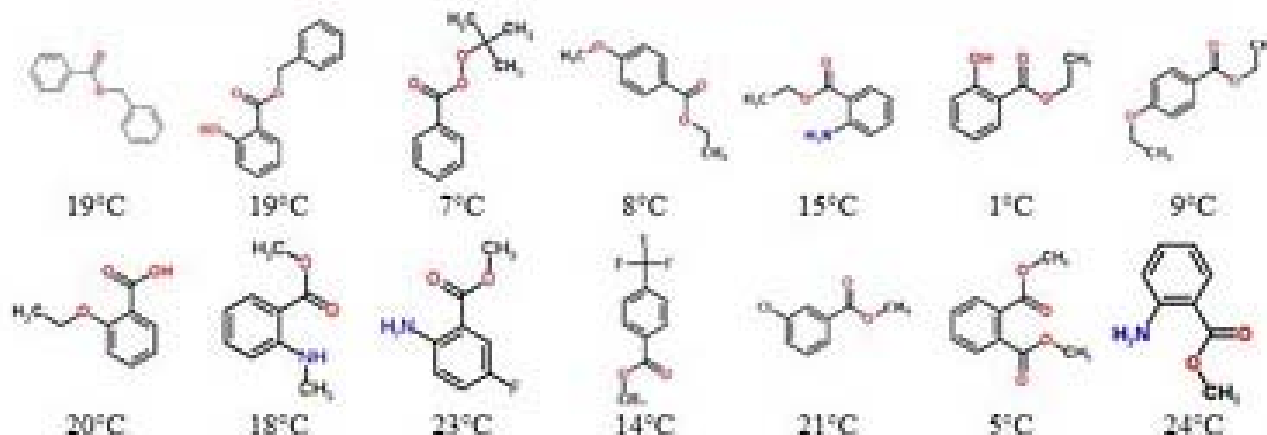
Outliers

Alfa Aesar

name	mp °C	source	SMILES
ethanol	-130.00	Alfa Aesar	CCO
ethanol	-114.40	commercial database	CCO
ethanol	-114.30	crowdsourced database	CCO
ethanol	-114.14	commercial database	CCO
ethanol	-114.00	academic website	CCO
ethanol	-114.00	chemical vendor	CCO

The average melting point of ethanol is -116.81 °C

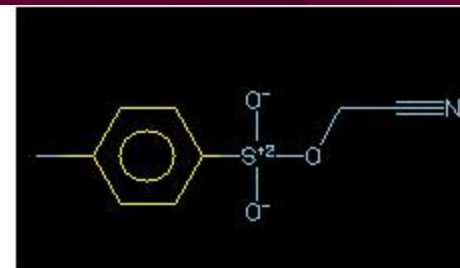# Inconsistencies and SMILES problems within MDPI dataset

name	mp C	Error C
androstane-3,17-dione	132	47.5
androstane-3,17-dione	179.5	47.5
Mephenytoin	136	74
Mephenytoin	210	74
N-cyclohexylbenzamide	145	17
N-cyclohexylbenzamide	162	17
9-Fluoro-6,7-dihydro-5,8-dimethyl-1-oxo-1H,5H-benzo[ij]quinoli:	194	75
9-Fluoro-6,7-dihydro-5,8-dimethyl-1-oxo-1H,5H-benzo[ij]quinoli:	269	75
5,6,7,8-tetrahydronaphthalene-1-carboxylic acid	148.5	11
5,6,7,8-tetrahydronaphthalene-1-carboxylic acid	159.5	11
N1-phenyl-3,3,3-trifluoro-2-(trifluoromethyl)propanamide	166	25
N1-phenyl-3,3,3-trifluoro-2-(trifluoromethyl)propanamide	191	25
N,N'-diphenylethanebis(thioamide)	134.5	16.5
N,N'-diphenylethanebis(thioamide)	151	16.5
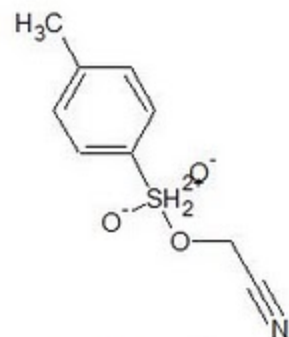
[S+2]([O-])([O-])(OCC#N)c1ccc(C)cc1
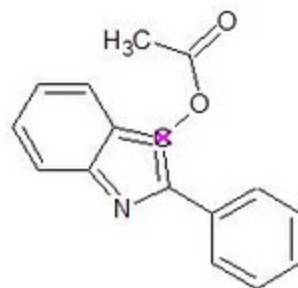
O=C(OC=1=C2C=CC=CC2=NC=1c1ccccc1)C

[S+2]([O-])([O-])(OCC#N)c1ccc(C)cc1

MDPI Dataset labeled with High Trust Level

Open Melting Point Datasets

ONSMP000: ([ONSCwiki](#)) 15591 full raw entries from Alfa Aesar containing duplicates and non numerical values

ONSMP001: ([ORU](#) ⬈) 12986 measurements as simple numeric values converted from mp ranges and other entries with non-numeric characters from Alfa Aesar (ONSMP000).

ONSMP002: ([ORU](#) ⬈) 8739 measurements derived from ONSMP001 with redundancies, salts, inorganics and organometallics removed. Silicon, phosphorus and boron containing organic compounds were retained. SMILES, CSIDs and links to the Alfa Aesar catalog are included.

ONSMP003: ([ORU](#) ⬈) 4450 measurements from [Karthikeyan 2005](#) ⬈. Includes SMILES and many descriptors.

ONSMP004: ([ORU](#) ⬈) 4084 measurements derived from ONSMP003 - includes compound names and CSIDs - excludes SMILES that did not properly render with OpenEye. 48 compounds were missing from ONSMP004 that were in ONSMP003 - these have been recovered but they do not have associated names or CSIDs: [ONSMP004a](#)

ONSMP005: ([ORU](#) ⬈) 277 measurements from [Bergstrom 2003](#) ⬈. Drug molecules separated as training and validation sheets. SMILES provided.

ONSMP006 ([ORU](#) ⬈) 277 measurements derived from ONSMP005 compiled into one sheet and both SMILES and CSIDs provided.

ONSMP007 (pending) curated Karthikeyan dataset ONS004 further curated by removal of all duplicate entries (with very different melting points)

ONSMP008 ([ONSCwiki](#)) 33 Duplicates (66 measurements) with a difference with more than 10C from the Karthikeyan dataset ONSMP003

ONSMP009 ([ONSCwiki](#)) 311 SMILES which could not be rendered correctly on ChemSketch from Karthikeyan dataset ONSMP003

ONSMP010 ([ONSCwiki](#)) 150 SMILES consisting of all EPI melting point data (via ChemSpider) from a 2011-03-04 snapshot of Cheminfo Validation sheet. 106 of these have at least one MP from another source. 10 of the 106 show a difference of at least 5C between the EPI and the other sources.
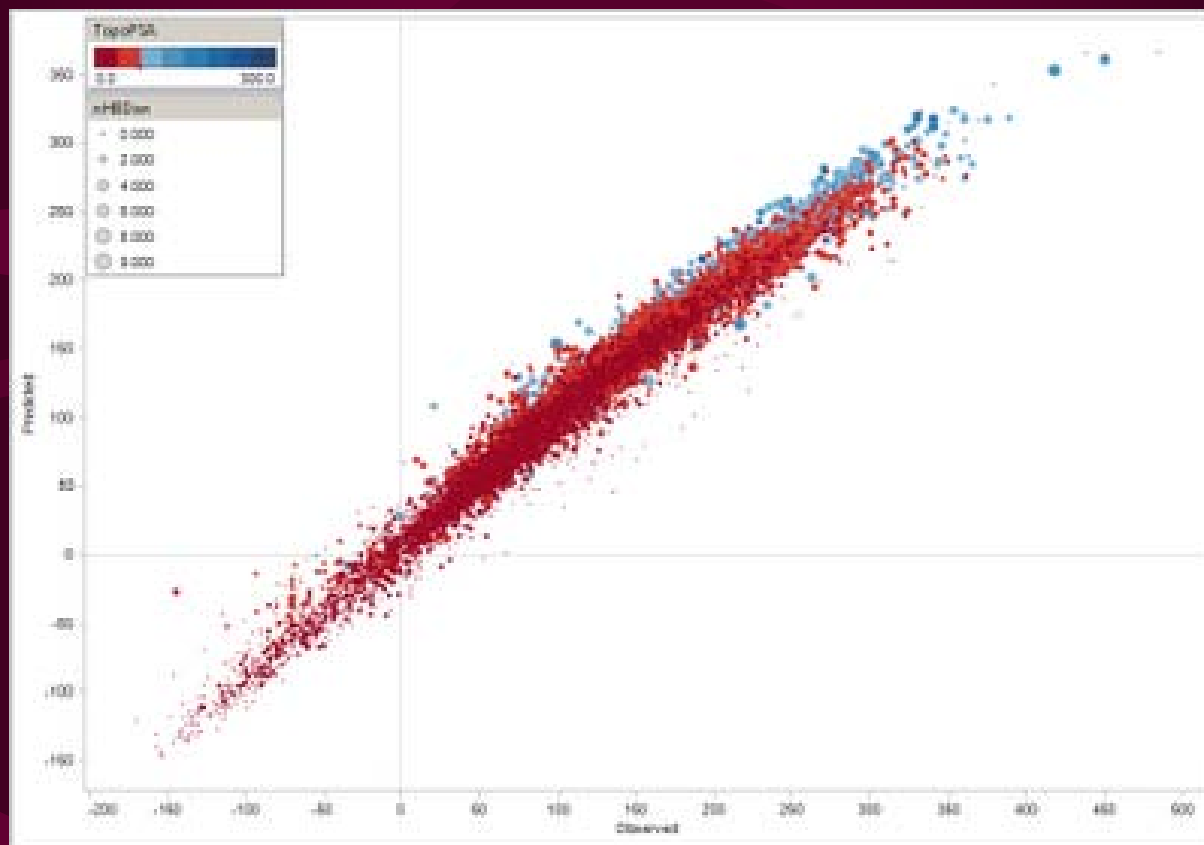
ONSMP011 ([ONSCwiki](#)) 335 measurements. A snapshot taken 2011-02-20 of the crowdsourced melting point data in the [ChemInfo Validation Sheet](#) ⬈.

ONSMP012 ([ONSCwiki](#)) 1286 measurements removed from the union of ONSMP002, ONSMP003, ONSMP006, and ONSMP011. Data were removed because they were either salts, had a large discrepancy in measurements (greater then 10C), were suspected erroneous measurements, were unneeded duplicates, or failed to produce CDK desscriptors, see [meltingpointmodel001](#).

ONSMP013 ([ORU](#) ⬈) 12634 highly curated (see ONSMP012 above) unique melting point measurements with CDK descriptor values based upon the union of ONSMP002, ONSMP003, ONSMP006, and ONSMP011.

http://onschallenge.wikispaces.com/Open+Melting+Point+Datasets

Open Random Forest modeling of Open Melting Point data using CDK descriptors
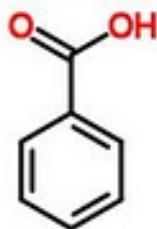## (Andrew Lang)

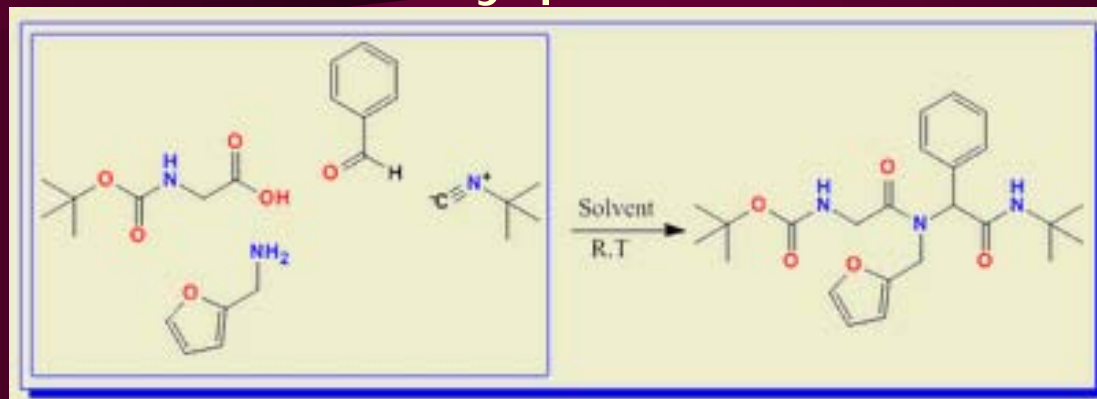## R2 = 0.78, TPSA and nHdon most important

Melting point prediction service

Using melting point for temperature dependent solubility prediction

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

Strategy for an Open Notebook:

First record then abstract structure

In order to be discoverable use Google friendly formats (simple HTML, no login)

In order to be replicable use free hosted tools (Wikispaces, Google Spreadsheets)

Crowdsourcing Solubility Data

http://onschallenge.wikispaces.com/
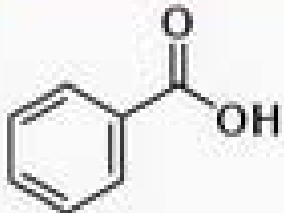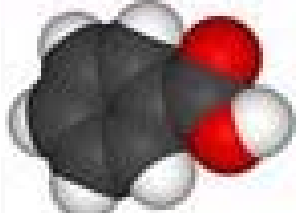
Data provenance:
From Wikipedia to...

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://bru.edu/cccda/s/solubility/allsolvents.php?solute=benzoic%20acid 🔗 Open Notebook Science Challenge Data.

...the lab notebook and raw data

Calculations Made Public on Google Spreadsheets

EXP208-WS1

File　Edit　Format　Insert　Tools　Form　Help

	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
					E	F	G	H	I	J	K	L	M
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

Interactive NMR spectra using JSpecView and JCAMP-DX

ARBITRARY UNITS

(6.58, 98)

Integral of: 4-Chlorobenzaldehyde-HNMR
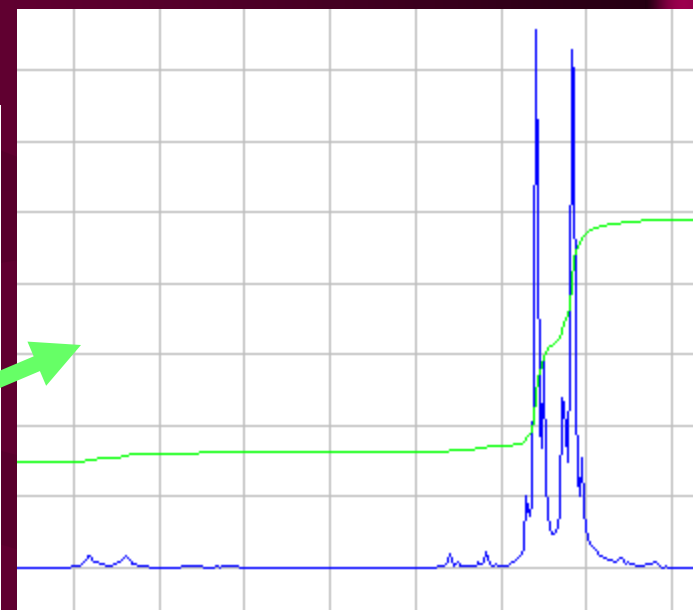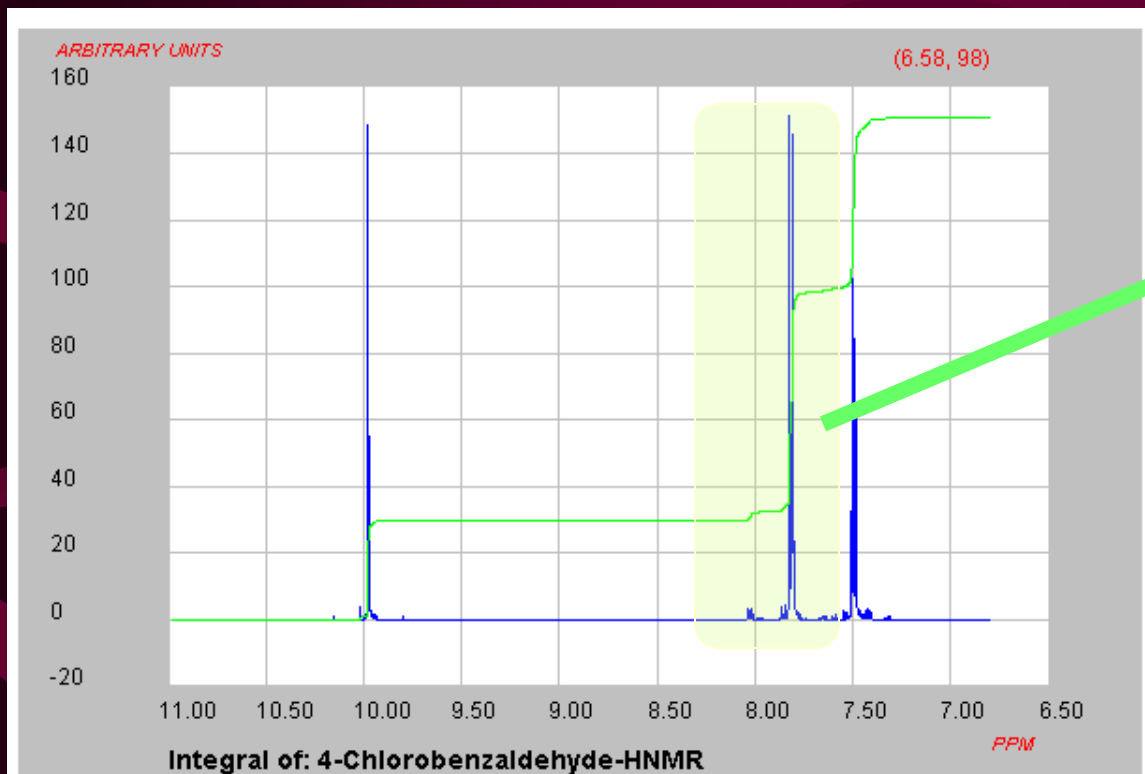
JSpecView version number is 1.0.20071009-2130

Created and maintained by Prof Robert John Lancashire

http://usefulchem.wikispaces.com/Exp208

Raw Data As Images

YouTube for demonstrating experimental set-up

The importance of raw data availability

4-nitrobenzaldehyde   hemiacetal
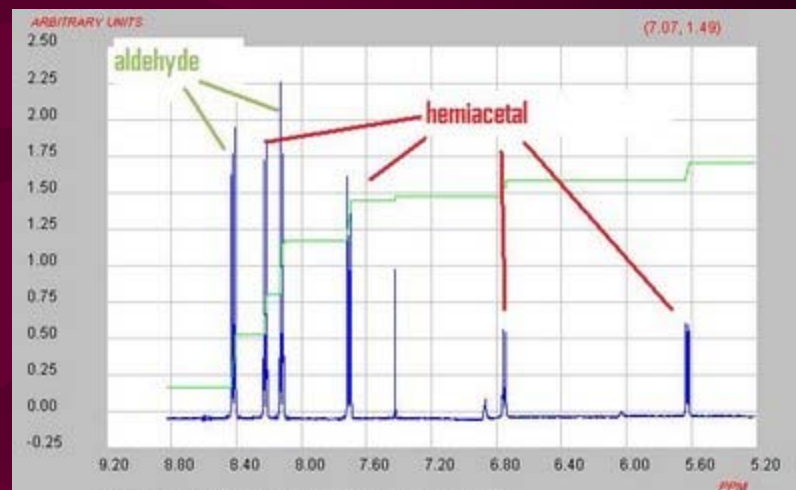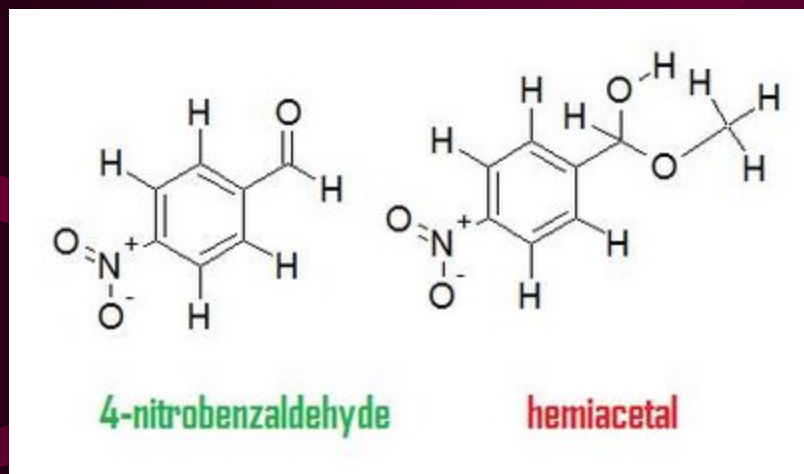
Missed in a prior publication on solubility for this compound

DETERMINATION OF THE SOLUBILITIES

An excess of finely powdered PNBA, BMTPP, TPPO, and PNPPPO was added to 5 ml of the appropriate solvent and shaken in a thermostatted bath for 24 h. Aliquots of 0.5 ml were withdrawn and analyzed after appropriate dilution. PNBA and TPPO were analyzed by GLC with internal standard methods (p-nitroacetophenone and p,p'-dimethoxybenzophenone, respectively). BMTPP and PNPPPO were analyzed by UV spectrophotometry in ethanol at 318 nm for the ylid ($\epsilon = 11{,}000$) and at 316 nm for the chalcone ($\epsilon = 29{,}000$).

Solubilities collected in a Google Spreadsheet

Google Docs BETA

Solubilites Sum

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

Web services for summary data

These results are from the Open Notebook Science Solubility Challenge as of January 15, 2011
A compilation of the results in book form can be obtained from Nature Precedings
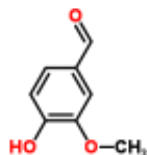
Solubility of vanillin in organic solvents.
Total Number of Results: 17
Total Number of Solvents: 9

	Solvent	Ave. (M)	Hits	SD	Link to Detailed Results
1.	1,2-dichloroethane	1.175	1	0.000	Solubility of vanillin in 1,2-dichloroethane is 1.175 M
2.	1-propanol	1.820	1	0.000	Solubility of vanillin in 1-propanol is 1.820 M
3.	THF	3.594	2	0.419	Solubility of vanillin in THF is 3.594 M
4.	acetonitrile	2.360	2	0.028	Solubility of vanillin in acetonitrile is 2.360 M
5.	butanone	2.138	1	0.000	Solubility of vanillin in butanone is 2.138 M
6.	ethanol	2.470	5	0.152	Solubility of vanillin in ethanol is 2.470 M
7.	methanol	4.160	3	0.026	Solubility of vanillin in methanol is 4.160 M
8.	toluene	0.302	1	0.000	Solubility of vanillin in toluene is 0.302 M
9.	water	0.070	1	0.000	Solubility of vanillin in water is 0.070 M

Permalink: http://old.oru.edu/cccda/sl/solubility/allsolvents.php?solute=vanillin

(Andrew Lang)

Web service calls from within a Google Spreadsheet for solubility measurement and prediction

Google docs — PredictionDemo — Public on the web

| File | Edit | View | Insert | Format | Form | Tools | Help |

	A	B	C	D	E
1	solute (name, CSID or SMILES)	solvent	predicted solubility (M)	measured solubility (M)	%error
2	benzoic acid	methanol	1.39	2.831	51
3	cinnamic acid	ethanol	0.843	1.03	18
4	ibuprofen	methanol	2.639	0.858	208
5	phenanthrene-9-carboxaldehyde	ethyl acetate	0.018	0.44	96
6	O=C(O)c1ccccc1	acetonitrile	0.464	No Records	#VALUE
7	phenanthrene-9-carboxaldehyde	benzene	0.066	0.66	90

http://onswebservices.wikispaces.com/

(Andrew Lang)

Integration of Multiple Web Services to Recommend Solvents for Reactions

(Andrew Lang)

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

by Andrew Lang et al.

★★★★★ (1 Rating)

Paperback, 130 pages

$8.20

Ships in 3–5 business days

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

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

Jean-Claude Bradley, Cameron Neylon, Anthony Williams, Rajarshi Guha, Bill Hooker, Andrew Lang, Tim Bohinski/David Bulger, Matthew Federici, Jennifer Hale, Jenna Mancinelli, Khalid Mirza, Marshall Moritz, Daniel Rein, Cedric Tchakounte, Hal Truong, Brent Friesen
Editors: Jean-Claude Bradley and Andrew Lang

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

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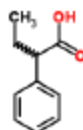
Molecular weight	164.201	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.38
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.09 g/cm³
SMILES	O=C(O)C(c1ccccc1)CC				
InChIKey	OFJWFSNDPCAWDK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (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]
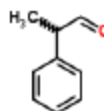
Compound Data

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)	pph (g/100g)
methanol	7.53	□	□

□ Solute is very soluble/miscible, conversion fail.

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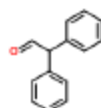
Compound Data

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)	pph (g/100g)
methanol	5.64	□	□

□ Solute is very soluble/miscible, conversion fail.

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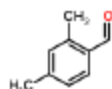
Compound Data

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)	pph (g/100g)
methanol	7.17	0.88	3128.10

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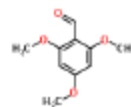
Compound Data

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)	pph (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)	pph (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]
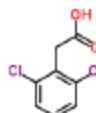
Compound Data

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)	pph (g/100g)
THF	3.08	0.30	120.05

3-mercaptopropionic acid $C_3H_4O_2S$ [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

Reaction Attempts

The UsefulChem Project

Find Reactions via Dropdown Filters

Component 1-pyrenebutyric acid ▾
Component 2,4-dimethylbenzaldehyde ▾
Component Select Reactant or Named Product ▾

Find Reactions via Substructure Search

SMARTS [   ]

◉ everything ○ reactants only ○ products only

[Substructure Search]

1 Reactions Found

Reaction ID UCEXP181-087V2

Researcher	Khalid Mirza
Reaction Type	Ugi
Solvent	methanol
Limiting Reactant	0.222 M
Precipitate	Reactants Insoluble
Comments	Protocol from Explan005 followed
Reference	http://usefulchem.wikispaces.com/Exp181
Solvent Selection	Optimal Solvent Prediction

OPEN NOTEBOOK SCIENCE CHALLENGE
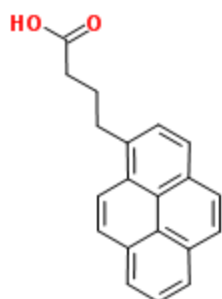
Reaction Attempts: Advanced Search

Compound: Any compound ▾
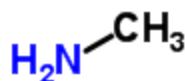Solvent: Any Solvent ▾
Reaction Type: Any Reaction Type ▾
Researcher: Any Researcher ▾
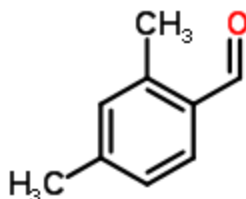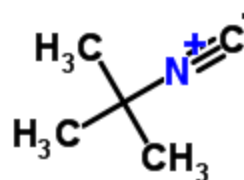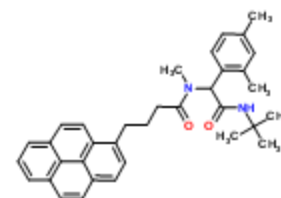
[Search]

1-pyrenebutyric acid + methylamine + 2,4-dimethylbenzaldehyde + t-butyl isocyanide → 21106206

Reaction Attempts Book

Reaction Attempts

By Andrew Lang, By Jean-Claude Bradley, By Tim Bohinski, By David Bulger, By Khalid Mirza, By Marshall Moritz, By Alicia Merchant, By Emily Messner, By Shannon Oseback, By Rikesh Parikh, By Mitesh Shah
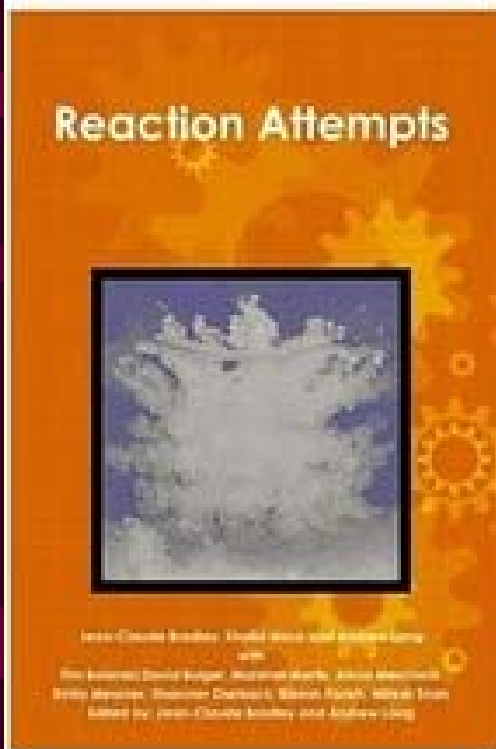
★★★★★ (1 Rating)

Paperback, 582 pages

$26.28

Ships in 3–5 business days

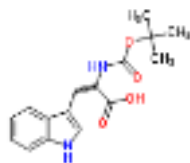A compilation of reaction attempts from the UsefulChem project.

Reaction Attempts Book: Reactants listed Alphabetically

Limiting Reactant 0.61 M
Precipitate No
Comments Protocol from Explan005 followed
Reference http://usefulchem.wikispaces.com/Exp131
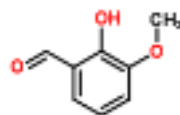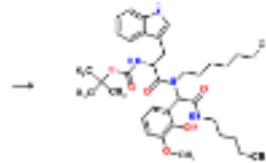
Boc-Trp-OH   1-heptylamine   o-vanillin   1-pentyl isocyanide   21106066

Reaction ID UCEXP148A-V1B153

Researcher Khalid Mirza/ Emily Messner
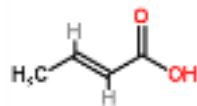**Reaction Type** Ugi
Solvent methanol
Limiting Reactant 0.398 M
Precipitate Yes but the aldehyde alone is not soluble in methanol
Yield 50.1 %
Comments Protocol from Explan005 followed
Reference http://usefulchem.wikispaces.com/Exp148
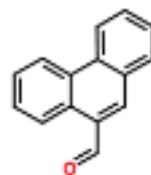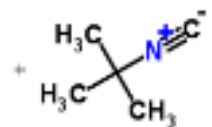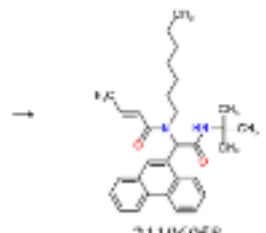
crotonic acid   1-heptylamine   phenanthrene-9-carboxaldehyde   t-butyl isocyanide   21106058

ONS Challenge Solubility Book cited for nanotechnology application

(a) 11.7 nm

(b) AuNP precipitates
Detached OA
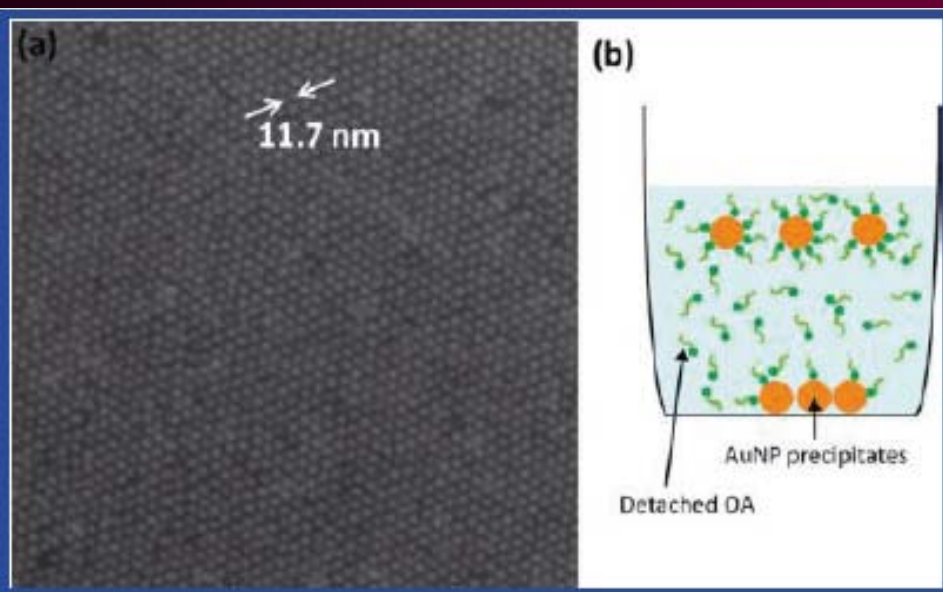
Although to our best knowledge there lacks literature value of OA solubility in the two solvents, the 10-fold better solubility of 1-otadecylamine (*sic*), the saturated version of oleylamine, in toluene than hexane is in line with our hypothesis.(33) This increased solubility caused the OA molecules that were originally attached to the AuNPs to gradually detach from the AuNPs, which is supported by our observations in poor AuNP stability and surface-pressure isotherms.

Langmuir

Enhanced Ordering in Gold Nanoparticles Self-Assembly through Excess Free Ligands

dx.doi.org/10.1021/la104786z

Cindy Y. Lau,[†] Huigao Duan,[‡] Fuke Wang,[‡] Chao Bin He,[‡] Hong Yee Low,[‡] and Joel K. W. Yang*,[‡]

Lulu.com Data Disks

Visualizing molecule-researcher connection maps reveals link between 2 Open Notebooks (Todd and Bradley)

http://usefulchem.blogspot.com/2010/12/visualizing-social-networks-in-open.html

(Don Pellegrino)

All ONS web services

Open Notebook Science Web Services

maintained by Jean-Claude Bradley and Andrew Lang

Solubility

Reactions

Chemical Information Validation

Melting Points

MyExperiment

Mendeley

NMR

Miscellaneous

http://onswebservices.wikispaces.com/

For all Formats of ONS Projects

Open Notebook Science Solubility Challenge

Live version

Book - HTML (entire ⇗ predictions only ⇗)
Spreadsheet - (SolubilitiesSum ⇗)
OData XML feed - (Solubilities ⇗)

Edition 3 (2010-02-11)

Book - PDF and shippable physical copy (LuLu ⇗)
Book - PDF only (Nature Precedings ⇗)
Data Archive - CD (LuLu ⇗)
Data Archive - ZIP (Drexel Chem Server ⇗) (Drexel Library iDEA Repository ⇗)
Data Archive - hosted interactive (Drexel Chem Server ⇗)
UsefulChem post ⇗

Reaction Attempts

Live version

Book - HTML (entire ⇗ selected reactants ⇗)
Spreadsheets - linked via RXIDs (Reactions ⇗ ReactionCompounds ⇗)
OData XML feeds - linked via RXIDs (Reactions ⇗ ReactionCompounds ⇗)

Edition 1 (2010-04-27) Data Source: UsefulChem Project

Book - PDF and shippable physical copy (LuLu ⇗)
Book - PDF only (Scribd ⇗)(Drexel Library iDEA repository ⇗) (Nature Precedings ⇗)
UsefulChem Data Archive - DVD (LuLu ⇗)
UsefulChem Data Archive - ZIP (Drexel Chem Server ⇗)
UsefulChem Data Archive - hosted interactive (Drexel Chem Server ⇗)
Reaction Attempts RXIDs spreadsheet - XLS (WebCite ⇗)
Reaction Attempts Reactants and Products spreadsheet XLS (WebCite ⇗)
UsefulChem Blog post ⇗

http://onsbooks.wikispaces.com

Conclusions

- Our current system of publication is not as transparent as it could be

- Open Notebook Science offers an efficient way to make research transparent and discoverable