

Mobile devices and “Generation App”

Antony Williams
ICIC Conference
October 2011

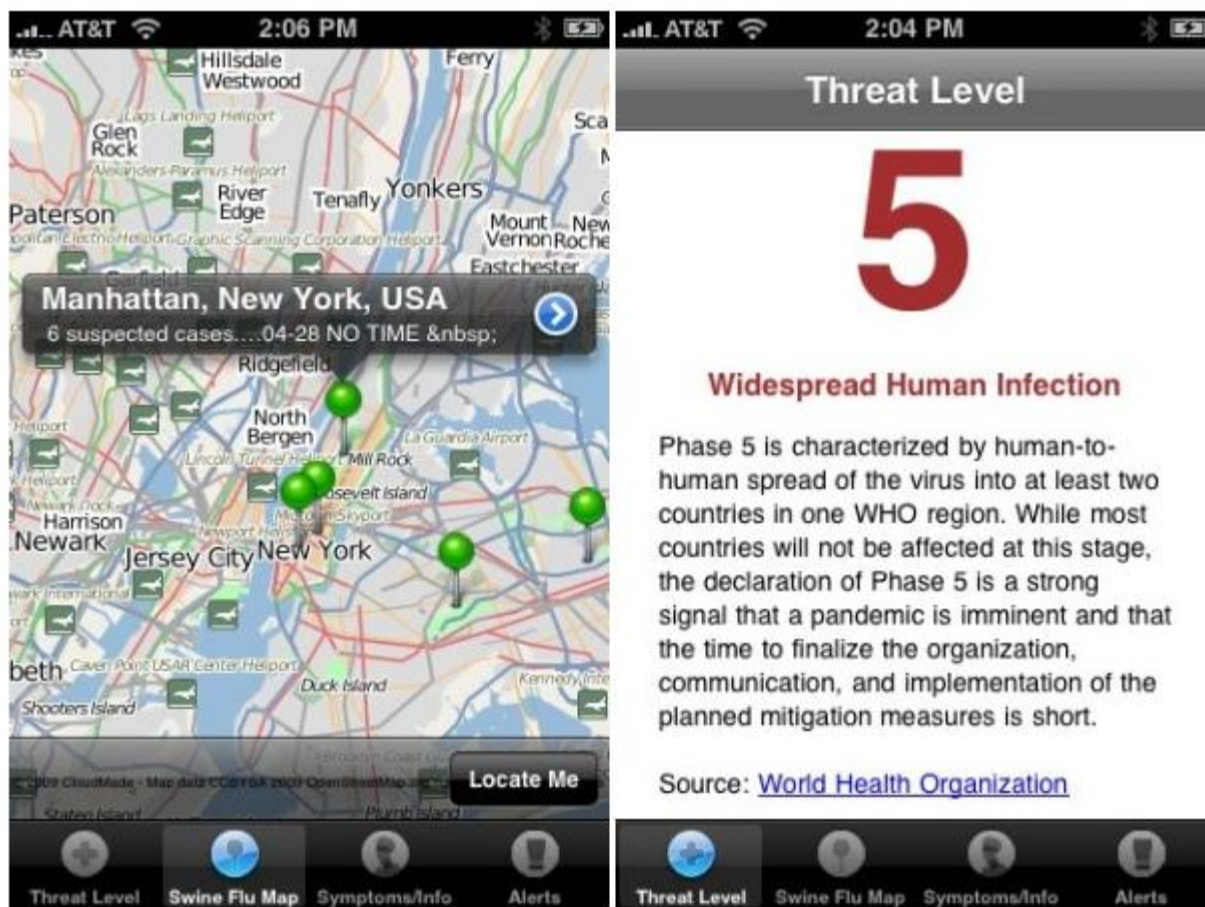
Mobilizing Chemistry

- We live in “Generation App”
- Mobile devices, apps, cloud-based services and databases provide “Chemistry in the Hand”
- Hundreds of apps are appearing: iOS (iPhone, iPads etc), Android, Blackberry etc.
- It’s not just Chemistry...Science has gone Mobile..

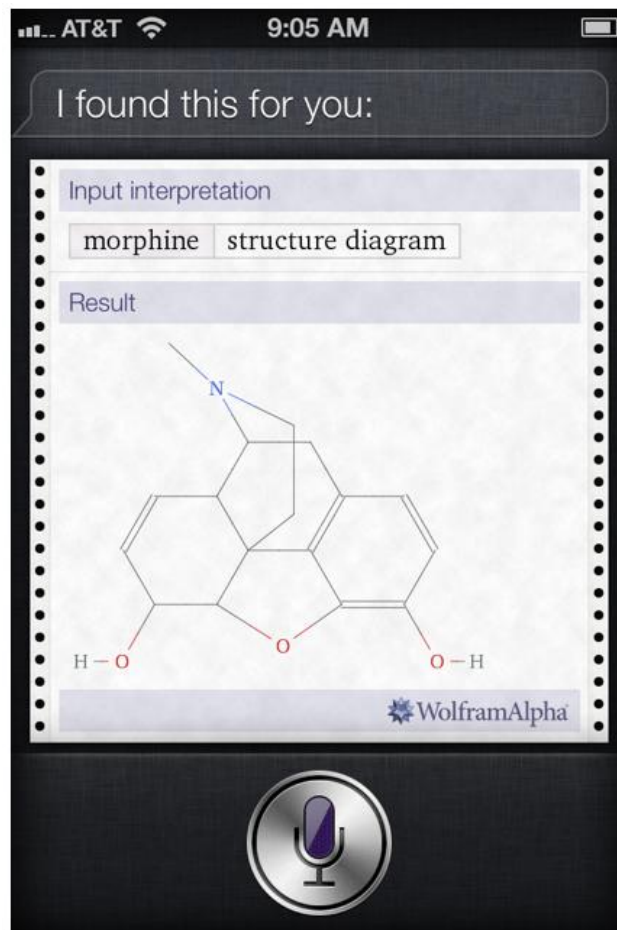
There's an "App for That"



There's an "App for That"



Siri Knows Chemistry



There's a lot of Mobile Chemistry!

- Categorization of chemistry apps. More later...

Contents

- 1 Apps for Chemistry
- 2 Green Chemistry
- 3 Publishers
- 4 Structure Drawing, Visualization and Chemical Databases
- 5 Chemical Calculators
- 6 Chemical Look-Ups
- 7 Chemical Compounds
- 8 Chemical Reactions
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- 10 Spectroscopy
- 11 Theoretical Chemistry
- 12 Periodic Tables

Scientific Publishers Apps

- Scientific publishers release apps to:
 - Provide mobile access to content
 - Search and deliver content to its registered users
 - Greater accessibility means greater readership
 - Revenue generation UNLIKELY via sales of Apps. Revenue comes from the content

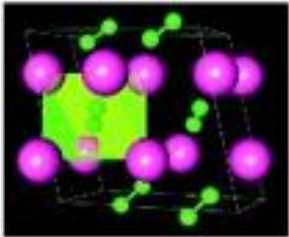
Scientific Publisher Apps (ACS)

<http://tinyurl.com/ykaprhf>

ACS ASAPs Filter

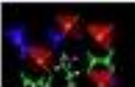
February 02, 2010

Nature of N–N Bonding within High-Pressure Noble-Metal Pernitrides an...
Michael Wessel and Richard Dronskowski



47 minutes ago J. Am. Chem. Soc.

Mixed Anion (Phosphate/Oxalate) Bonding to Iron(III) Materials
Fiona R. Kizewski, Paul Boyle, Dean Hesterberg and James D. Martin



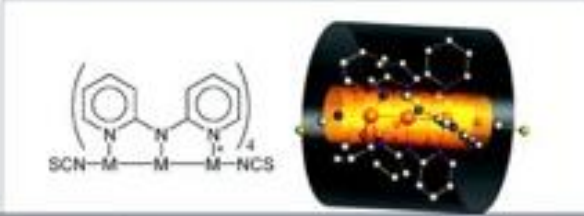
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Smallest Electrical Wire Based on Extended Metal-Atom Chains
Te-Wei Tsai, Qian-Rui Huang, Shie-Ming Peng and Bih-Yaw Jin
Department of Chemistry and Center for Theoretical Sciences, National Taiwan University, Taipei, Taiwan, Republic of China

J. Phys. Chem. C
DOI: 10.1021/jp907893q
Publication Date (Web): February 4, 2010
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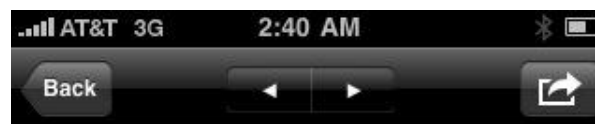
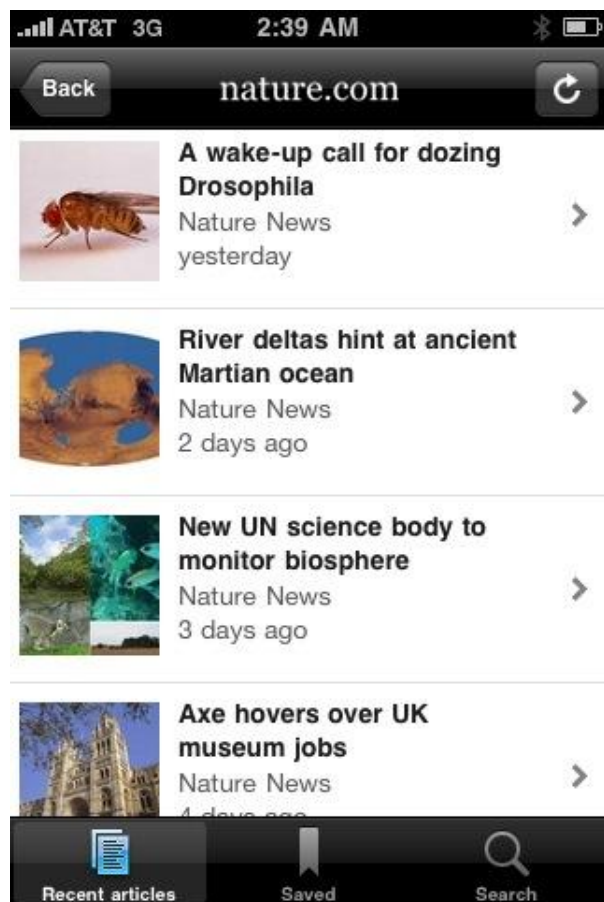
Abstract



Full Text ⏪ ⏩

Scientific Publisher Apps (Nature)

<http://www.nature.com/mobileapps/>



New UN science body to monitor biosphere

Emma Marris



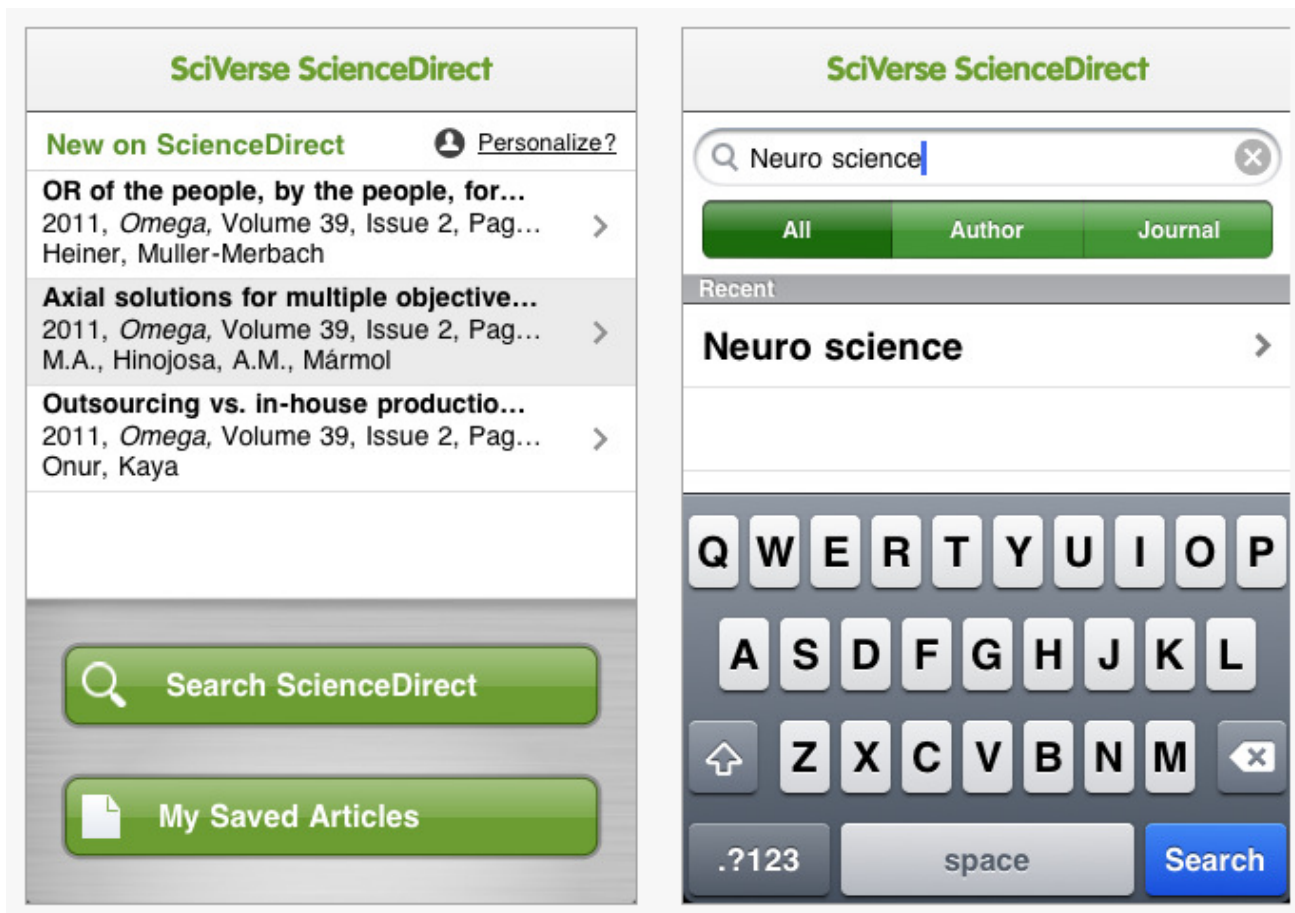
All creatures great and small: A newly approved global science organization to oversee life on earth will have its work cut out for it.

Credit: Cesar Paes Barreto

Representatives from close to 90 countries

SciVerse ScienceDirect

<http://tinyurl.com/3czq37y>



Sciverse Scopus

<http://www.info.sciverse.com/scopus>



Search

Search

Search for

In

Title - Abstract - Keywords

Select specific search terms to narrow your search:

- Use search terms that are specific rather than general to make your search as targeted as possible
- Select the field you want to search in (e.g. Author name or Journal title)
- You can use the following operators:
 - Boolean (AND, OR, AND NOT)
 - Wildcards (* and ?)

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Results

Options

1511 results for "Neuro science" Showing 50 results

Neuro-fuzzy based constraint programming
(2010) Yazdi, H.S., Hosseini, S.E., Yazdi, M.S.
Cited 0. *Applied Mathematical Modelling*

Undergraduate neuroscience faculty: Results fr...
(2010) Hardwick, J.C., Smith, J.S.
Cited 0. *Journal of Undergraduate Neuroscience Education*

Expressing and characterization of m lin-41 in...
(2010) Yu, G., Yang, Y., Tian, G.
Cited 0. *Journal of Molecular Histology*

Central and Peripheral Cytokines Mediate Immu...
(2010) Besedovsky, H.O., del Rey, A.
Cited 0. *Neurochemical Research*

Enabling Persons with Acquired Brain Injury an...
(2010) Lancioni, G.E., Singh, N.N., O'Reilly, M.F.,...

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Science App

http://www.aaas.org/news/releases/2010/1108science_app.shtml



Online Tools for Publications



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Citations to my articles



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Title / Author	Cited by	Year
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Antony Williams, PhD

Vice President, Strategic Development, Royal Society of Chemistry
Wake Forest, North Carolina, United States

Research field: Chemistry
Semantic Web for Chemistry
Cheminformatics
Spectroscopy
Analytical Data Processing
Nuclear Magnetic processing
Systematic Nomenclature

Publication Statistics

Graphed by cumulative total

All Time Past Year Past Month Past Week

Readers (499) Downloads (39)

Publications

▼ [Book \(4\)](#)

Williams Antony J. (2010) Enhancing Learning with Online Resources, Social Networking, and Digital Libraries, 23-39. In *American Chemical Society*.
<http://dx.doi.org/10.1021/bk-2010-106...>

Cameron Neylon, Rajarshi Guha, Antony J. Williams, Bill Hooker, Andrew S. I. D. Lang, Brent Friesen, Tim Bohinski, David Bulger, Matthew Federici, Jenny Hale, Jenna Mancinelli, Khalid B. Mirza, Marshall J. Moritz, Daniel Rein, Cedric Tchakounte & Hai T. T. Jean-Claude Bradley (2010) Open Notebook Science Challenge: Solubilities of Organic Compounds in Organic Solvents. In *Nature Precedings*.
<http://precedings.nature.com/document...>

51 Contacts

[See all](#)

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Andrew Lang

Khalid Mirza

Elizabeth Brown

Evan Curtin

Ramani Jayesh

Co-author (222)
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Antony J. Williams (Antony Williams)

Royal Society of Chemistry

Publications: 124 | Citations: 196 | G-Index: 9 | H-Index: 7

Interests: [Engineering](#), [Applied Chemistry](#), [Computational Chemistry](#)

Collaborated with 222 co-authors from 1986 to 2011; Cited by 366 authors

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[Journal \(35\)](#)

MAGN RESON CHEM

J HETEROCYCL CHEM

J CHEM INF MODEL

Cheminform

LANGMUIR

[Keyword \(125\)](#)

[Publication \(124\)](#) BibTeX

[Online chemical modeling environment \(OCHEM\): web platform for data storage, model development and publishing of chemical information](#)

Iurii Sushko, Sergii Novotarskyi, Robert Kömer, Anil Kumar Pandey, Matthias Rupp, Wolfram Teetz, Stefan Brandmaier, Ahmed Abdelaziz, Volodymyr V. Prokopenko, Vsevolod Y. Tanchuk, Roberto Todeschini, Alexandre Vamek... [Antony Williams...](#) [View All](#)

Published in 2011

“Papers” for Managing Publications



“Mendeley” for Managing Publications

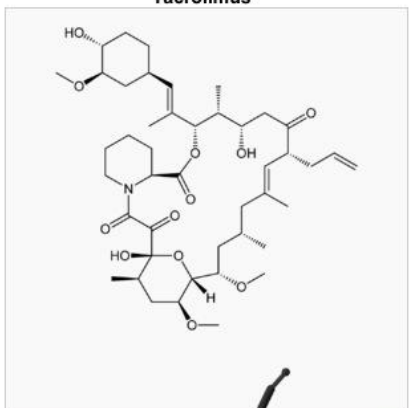


Wikipedia Chemistry



Tacrolimus

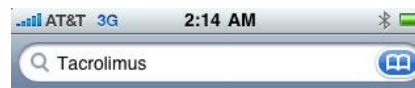
Tacrolimus

A screenshot of a mobile browser showing search results for Tacrolimus. The search bar contains "Tacrolimus". Below the search bar is a table with the following data:

Identifiers	
CAS number	104987-11-3
ATC code	D11AH01 L04AD02
PubChem	CID 656830
DrugBank	DB00864
ChemSpider	4976056

Chemical data	
Formula	C ₄₄ H ₆₉ NO ₁₂
Mol. mass	804.018 g/mol
SMILES	eMolecules & PubChem

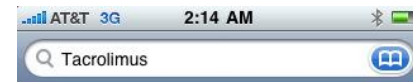
Pharmacokinetic data	
Bioavailability	20%, less after eating food rich in fat
Protein binding	75-99%
Metabolism	Hepatic CYP3A4
Half-life	11.3 h (range 3.5-40.6 h)
Excretion	Mostly faecal



Tacrolimus (also **FK-506** or **Fujimycin**) is an immunosuppressive drug whose main use is after allogeneic organ transplant to reduce the activity of the patient's immune system and so lower the risk of organ rejection. It reduces interleukin-2 (IL-2) production by T-cells. It is also used in a topical preparation in the treatment of severe atopic dermatitis (eczema), severe refractory uveitis after bone marrow transplants, and the skin condition vitiligo. It is a 23-membered macrolide lactone discovered in 1984 from the fermentation broth of a Japanese soil sample that contained the bacteria *Streptomyces tsukubaensis*.

Show History

Show Availability



Show History

Show Availability

Show Pharmacology

Show Indications

Show Side effects

Show Contraindications and precautions

Show References

Show External links

THEODORE GRAY THE Elements

The periodic table displays 118 elements, each with a small photograph of a sample. The elements are arranged in rows and columns, with their atomic numbers and symbols. The title 'THEODORE GRAY THE Elements' is prominently displayed in the center. The background is dark, and the text is white and light gray. Some elements have handwritten labels in various colors (e.g., '91', '91A', '9X', '911', '912', '913', '914', '915', '916', '917', '918').

I GIVE YOU HERE THE UNIVERSAL CATALOG OF EVERYTHING YOU CAN DROP ON YOUR FOOT: THESE ARE THE ELEMENTS, THE BUILDING BLOCKS OF YOUR WORLD AND THE BASIC STUFF OF ALL THAT IS HERE OR THERE OR ANYWHERE. ENJOY! TOUCH ANY ELEMENT TO SEE MORE, THEN GO TO ITS SECOND PAGE FOR ROTATABLE SAMPLES AND A STORY OR TWO.

29 Copper

Copper is wonderful stuff. Just wonderful. Many other elements have some kind of a gotcha about them: maybe they are great in every way except they're poisonous, or they would be perfect except they explode when they touch water. Copper has no gotcha—it's just nice stuff all around.

Copper can be toxic, but it takes special effort—eating large amounts of copper sulfate, or routinely eating acidic foods that have been stored in copper containers for a long time.

Extended contact with copper objects rarely causes harm. In fact, copper has antimicrobial properties that make it useful in hospitals for doorknobs and other surfaces on which infections may be passed (though claims of the mystical healing powers of copper bracelets are, of course, nonsense).

Copper is soft enough to be worked using hand tools or modest power tools, yet hard enough to be made into very useful things, especially when alloyed with tin (50) or zinc (30) to create, respectively, bronze or brass. You can even find copper in native metallic form in several places around the world, making it one of the first useful metals (hence "the Bronze Age," which I guess sounds better than "the Copper Alloy Age").

Copper is the only reasonably priced metal that isn't gray, quite a remarkable fact if you think about it. Every single one of the hundred-odd metallic elements is some shade of gray, except gold (79) and copper. Not surprisingly, copper has been used in jewelry since antiquity, where its only real disadvantage is that it tarnishes slowly, while gold remains bright forever (at six thousand times the price).

Unbeknownst to the ancients, copper has another nice attribute: the second-highest electrical conductivity of any metal. Vast quantities of copper are used for electrical wiring, making it as vital to the modern age as it was to the Bronze Age.

It may not be as pretty as copper, but I will always have a special place in my heart for the next element, zinc.



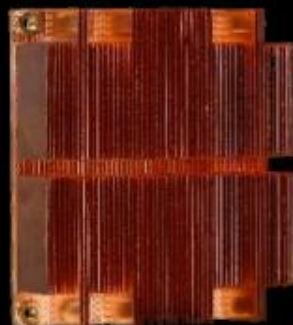
Half-Persian 4-in-1 weave chain made from copper electrical wire.



Brass, a copper alloy, has been used in jewelry from ancient times to the modern mall.



Copper electro-winning nodule.



Solid copper heat sink for a CPU chip.



Copper electrical cable thick enough to carry 400 amps.



Coppersmiths make cups and pitchers by hand from copper sheet.

Bronze is used in art and statuary the world over. This is a cheap Chinese trinket in heavy bronze.



Cu

29



Copper



Atomic Radius
145pm

Crystal Structure
Face Centered
Cubic

Electron Shells
[Ar]3d¹⁰4s¹

Atomic Weight 63.546

Density 8.920 g/cc

Melting Point 1084.62°C
1984.32°F

Boiling Point 2927°C
5301°F

Electronegativity 1.90

% in Universe 0.0000060%

% in Sun 0.000070%

% in Crust 0.0068%

% in Ocean 0.00000030%

% in Humans 0.0001%

computational knowledge from

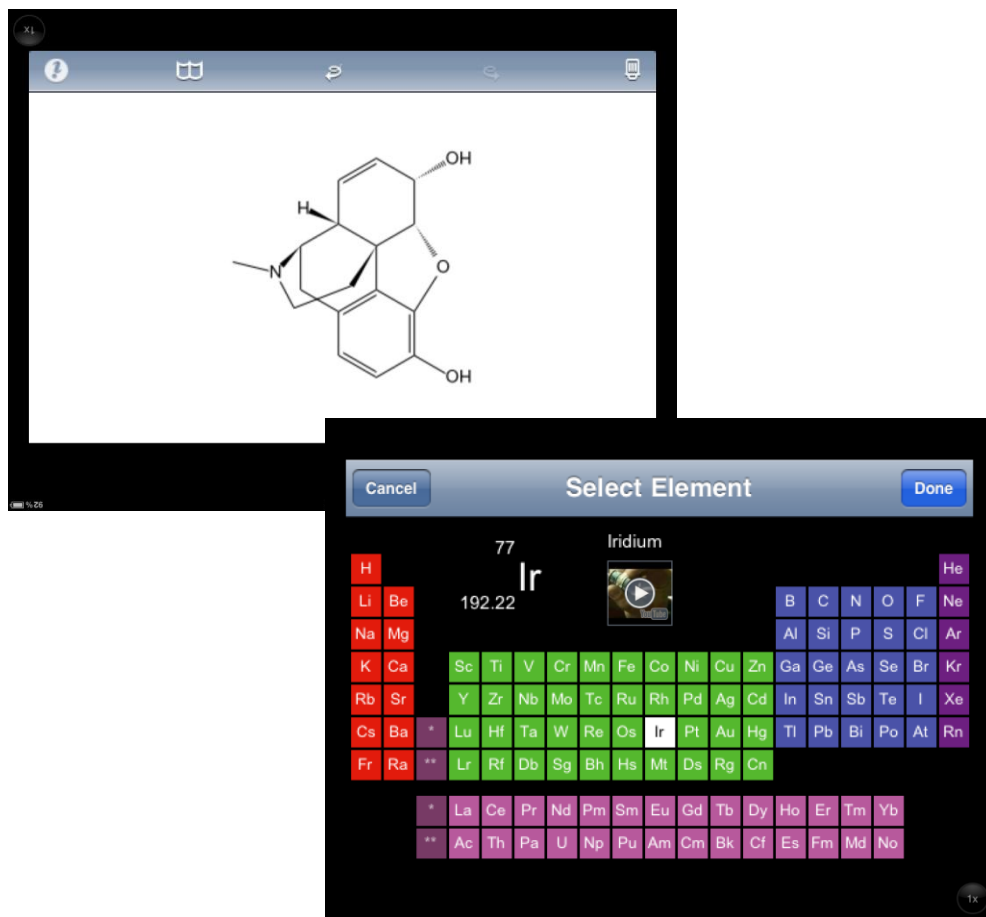
 **WolframAlpha**



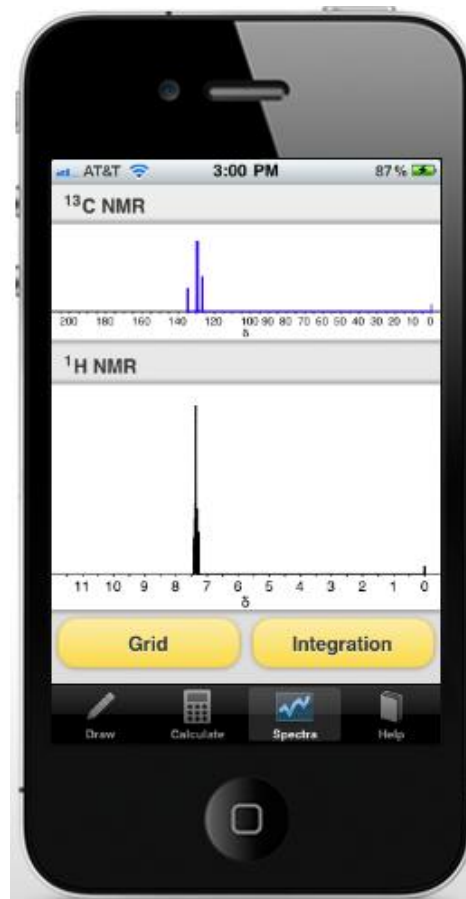
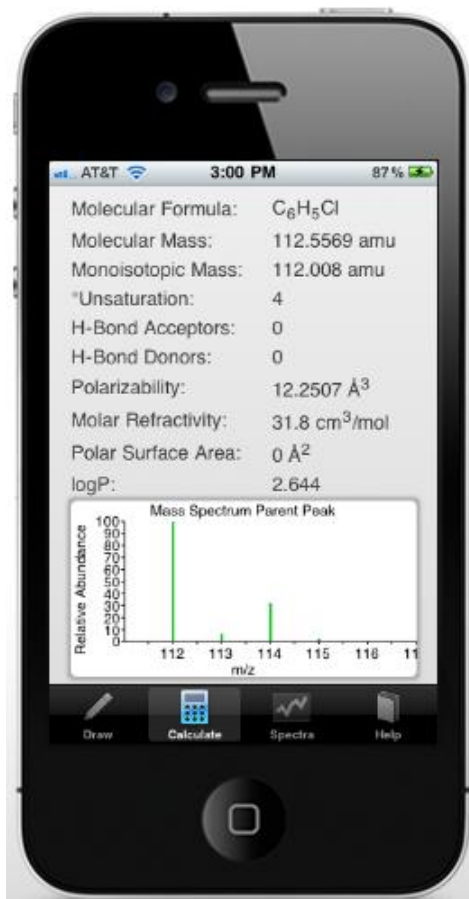
Structure Drawing as an entry point

- Structure entry as an entry point to:
 - Calculations (formula, mass)
 - Predictions (local or server-based)
 - Systematic name generation, logP, pKa, NMR prediction, etc.
 - Database lookup
 - On device dictionaries (because space doesn't matter!)
 - Internet-hosted databases (because the latest content does matter)

Chemical Structure Drawing ChemJuice

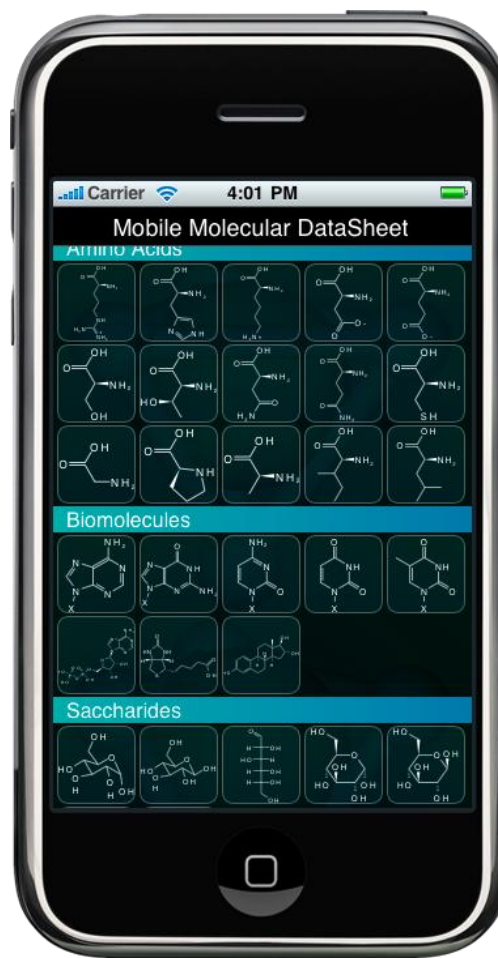


ChemDoodle Mobile

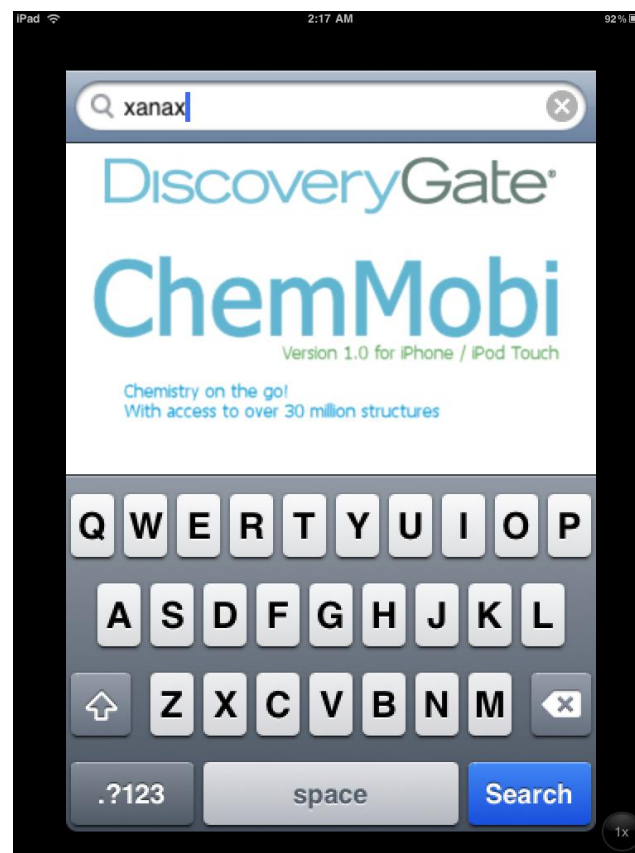
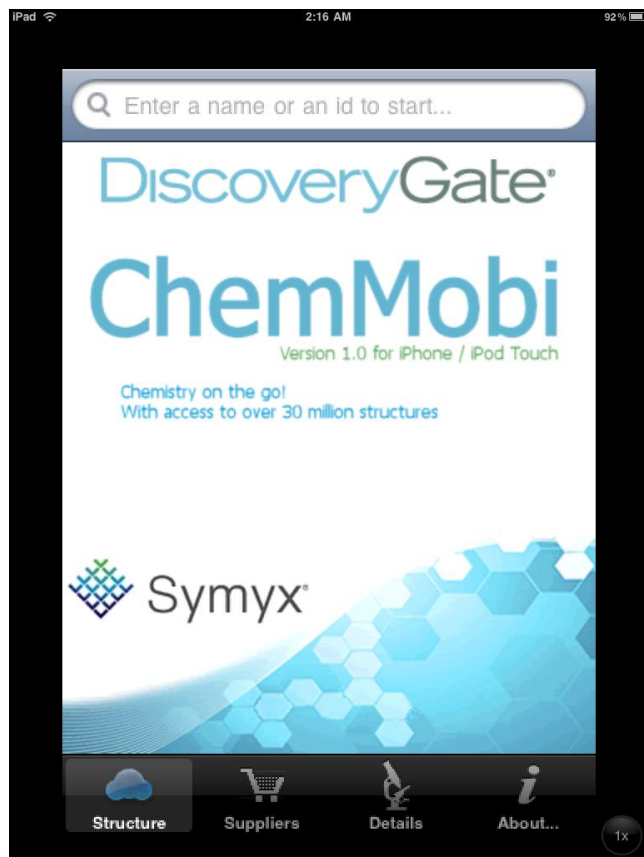


Chemical Structure Drawing

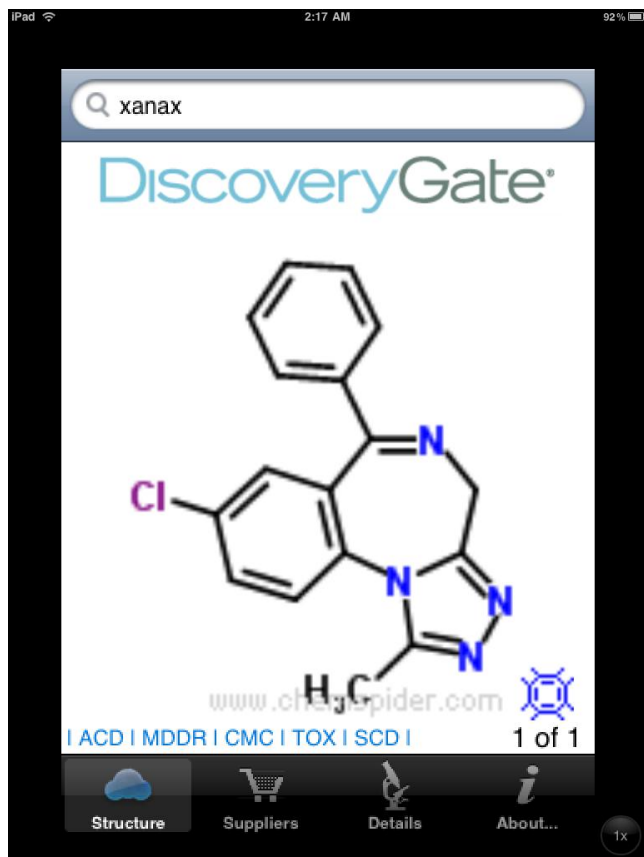
Mobile Molecular Datasheet



1st Structure Lookup of ChemSpider



1st Structure Lookup of ChemSpider



All Preferred

Filter

A

- AB Chem. Inc.
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Property	Value
ChemSpider ID	2034
Empirical Formula	C ₁₇ H ₁₃ ClN ₄
Molecular Weight	308.7649
Nominal Mass	308 Da


AT&T 3G 2:06 AM



Property	Value
ACD/LogP	2.499
ACD/LogD (pH5.5)	2.5
ACD/BCF (pH5.5)	46.67
ACD/KOC (pH5.5)	544.74
ACD/LogD (pH7.4)	2.5
ACD/BCF (pH7.4)	46.71
ACD/KOC (pH7.4)	545.23
# of Rule of 5 Violations	0
#H bond acceptors	4
#H bond donors	0
#Freely Rotating Bonds	1
Polar Surface Area	43.07

2nd Structure Lookup of ChemSpider

AT&T 3G 2:07 AM



Legend: ** approved by experts; * approved by users; -> redirected by users; ->* redirect approved

Alprazolam ** [\[wiki\]](#)
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Alprax **
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Xanor ** [\[wiki\]](#)
Staccato-alprazolam **
Alprazolam (JP15/USP) **
Alprazolam [USAN:BAN:INN:JAN] **
ZINC00000903 **
U-31889 **
4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-1-methyl-5-phenyl- **

Navigation icons: back, forward, home, search, tabs

AT&T 3G 2:08 AM

[Alprazolam - Wikipedia, the free encyclopedia](#)
Alprazolam, also known under the trade names Xanax, **Xanor**, **Alprax**, and Niravam, is a highly potent short-acting drug of the ...
[History](#) - [Indications](#) - [Side effects](#)
en.wikipedia.org/wiki/Alprazolam - [Options](#) ▾

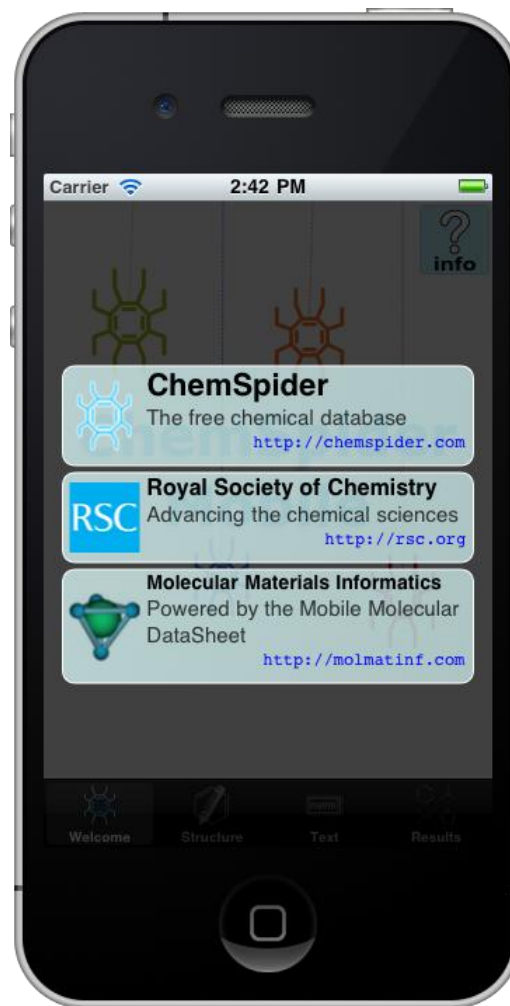
[Alprazolam Information from Drugs.com](#)
Jun 24, 2009 ... **Alprazolam** is used to treat anxiety disorders, panic disorders, and anxiety. Includes **alprazolam** side effects, ...
www.drugs.com/alprazolam.html - [Options](#) ▾

[Xanax \(Alprazolam\) Drug Information: Uses, Side Effects, Drug ...](#)
Aug 1, 2009 ... Learn about the prescription medication Xanax (**Alprazolam**), drug uses, dosage, side effects, drug interactions, ...
www.rxlist.com/xanax-drug.htm - [Options](#) ▾

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Buy **Alprazolam!** No Prescription Meds! Quality

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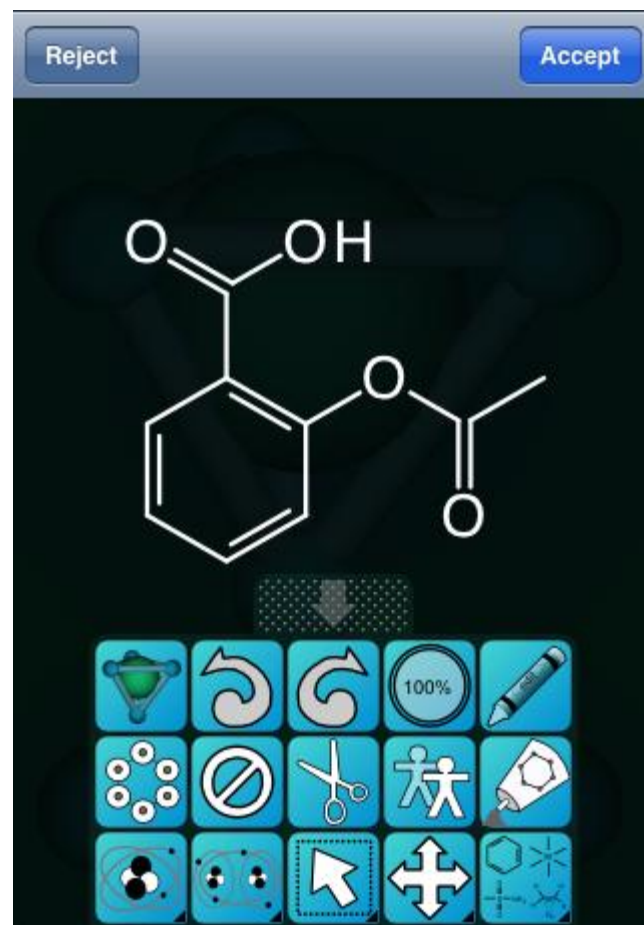
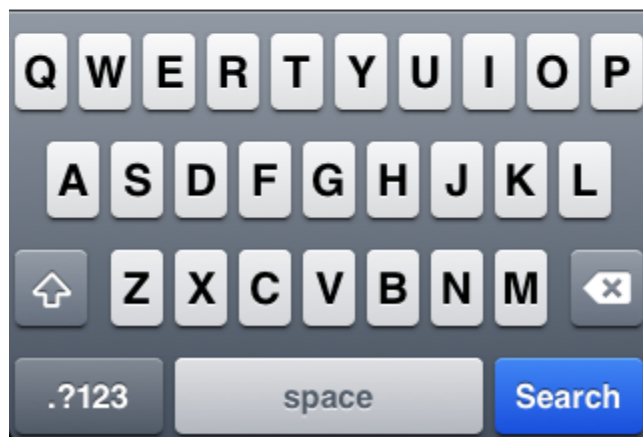
ChemSpider Mobile



Text and Structure Searching

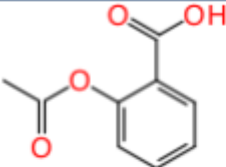
Cancel Search

aspirin



Exact and Skeleton Search

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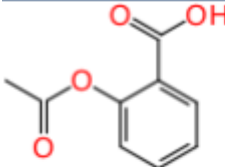


Aspirin

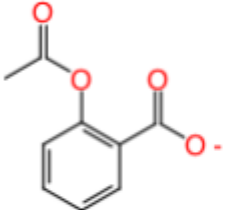
 

Structure Text Results

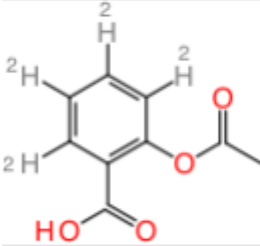
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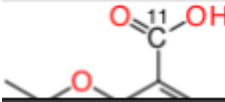
Aspirin





acetylsalicylate



2-Acetoxy(~2~H_4_...



2-(acetyloxy)(carboxy...

Structure Text Results

Open in Browser

- Coming soon:
 - Substructure searching
 - Similarity searching

ChemSpider | Aspirin | C₉H₈O₄

www.chemspider.com/...

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 ChemSpider
The free chemical database

RSC | Advancing the Chemical Sciences

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Aspirin

ChemSpider ID: 2187
Molecular Formula: C₉H₈O₄
Molecular Weight: 180.152 Da
Systematic name: 2-(acetyloxy)benzoic acid
SMILES and InChI

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Chemical Reactions

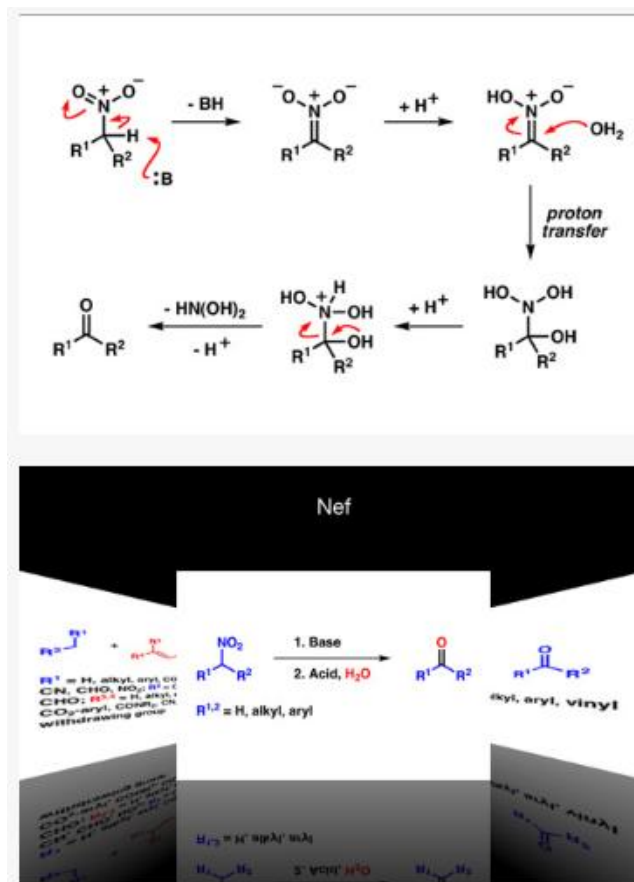
- Chemical reactions are very amenable to serving up on mobile applications
- What is available now?
 - Teaching basics of chemical reactions
 - Look-ups against reaction databases
 - Reaction mechanisms

Named Reactions

<http://www.synthetiqsolutions.com/named-reactions/>



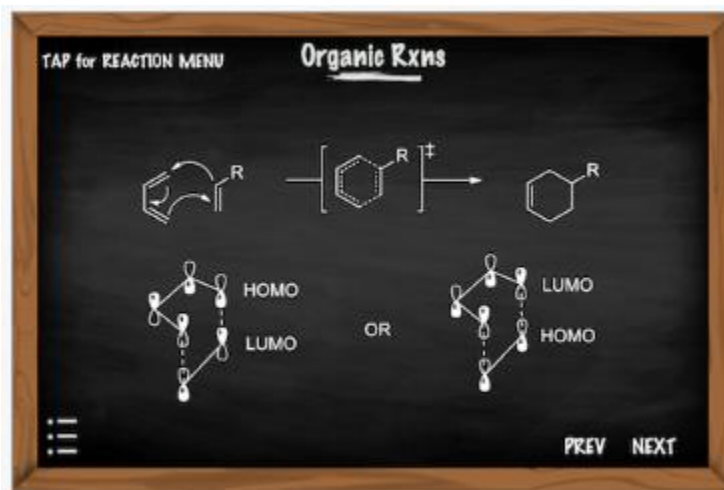
Reactions	
Info	
Q Search	Q
A	B
Aldol	C
	D
Alkene metathesis	F
	G
B	H
Bamford-Stevens	J
	L
C	M
Claisen condensation	N
	O
Curtius rearrangement	P
	R
D	S
Diels-Alder	T
	W
F	



Organic Named Reactions

<http://tinyurl.com/3d54fvv>

Organic
Named
Reactions



ReactionFlash

<http://tinyurl.com/3nt54w6>



Carrier 15:20

Filter All Categories All Levels

P

Prins-Pinacol Rearrangement

R

Reformatsky Reaction

Reformatsky-Blaise Zinc Alkylation

Robinson Annulation

S

Sandmeyer Reaction

Schiemann Aromatic Fluorination

Schmidt Reaction

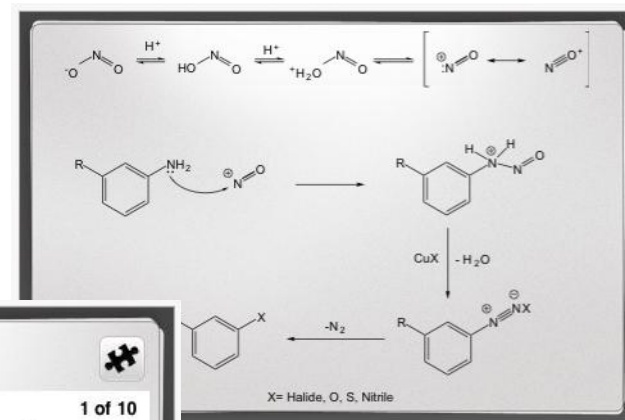
Reactions Favorites Search Quiz Settings

Sandmeyer Reaction

1 of 10

85% Stage #1: With hydrogen bromide; sodium nitrite in water - T=5°C; 0.17 h;
Stage #2: With hydrogen bromide; copper(I) bromide in water - T=20°C;
4 h Heating;
Tetrahedron, 2001, vol. 57, # 23 p. 4967 - 4976

Mechanism reaxys Examples

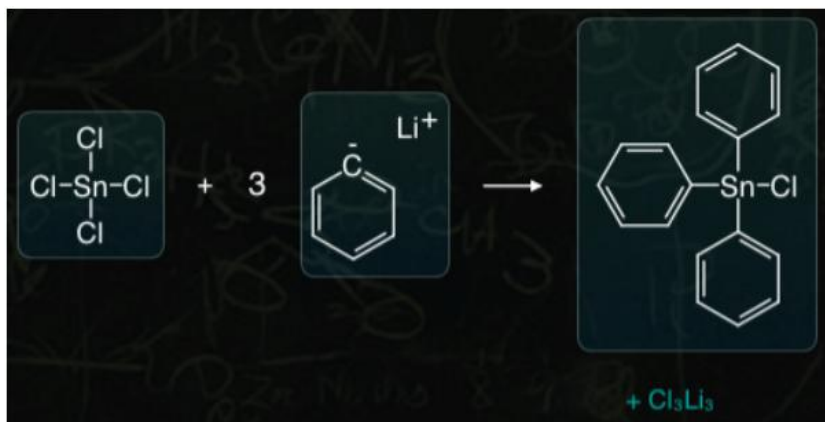










Sandmeyer Reaction

Score 0 POINTS 07:21 Submit

Reaction101

<http://molmatinf.com/reaction101.html>



Baylis Hillman vinyl alkylation	▶	Baylis Hillman vinyl alkylation	▶
Baylis-Hillman vinyl alkylation	▶	Baylis-Hillman vinyl alkylation	▶
Benzidine rearrangement	▶	Benzidine rearrangement	▶
Beta HX elimination Zaitsev elim...	▶	Beta HX elimination Zaitsev elim...	▶
Birch reduction	▶	 →  Birch reduction	▶
Borch reductive amination	▶	 →  Birch reduction	▶
Bromination of aliphatic nitro co...	▶	 →  Birch reduction	▶
Buchwald Hartwig cross coupling	▶	 →  Birch reduction	▶
Carboxylic acid addition to alkyn...	▶		
Carboxylic acid addition to alkyn...	▶		
Catalytic hydration of alkenes	▶		
Catalytic hydrogenation of arom...	▶		
Catalytic hydrogenation of arom...	▶		

Cancel Select Cancel Select

Yield 101

<http://molmatinf.com/yield101.html>



Chemical reaction interface showing the synthesis of 1-(4-hydroxyphenyl)ethane-1-ol from 1-phenylethanol and ethyne.

1-phenylethanol (122.16 g/mol):
Equiv: 1
Mass: 5 g
Moles: 0.0409285 mol
Density:
Conc:
Primary: *

Ethyne (26.04 g/mol):
Equiv: 1
Mass: 1.06567 g
Moles: 0.0409285 mol
Density:
Conc:
Primary:

1-(4-hydroxyphenyl)ethane-1-ol (148.20 g/mol):
Equiv: 1
Mass: 3.5 g
Moles: 0.0236165 mol
Density:
Conc:
Yield: 57.7018 %

Chemical reaction interface showing the synthesis of 1-(4-hydroxyphenyl)ethane-1-ol from 1-phenylethanol and ethyne.

1-phenylethanol (122.16 g/mol):
Equiv: 1
Mass: 5 g
Volume:
Moles: 0.0409285 mol
Density:
Conc:
Primary: *

Ethyne (26.04 g/mol):
Equiv: 1
Mass: 1.06567 g
Volume:
Moles: 0.0409285 mol
Density:
Conc:
Primary:

Reaction Database Look-up

Mobile version | [Full version](#)



Keyword, Chemical Name, Author's Name

Search

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benzene

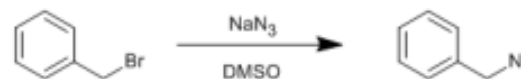
Search

27 hits found

[Nucleophilic substitution at benzyl halide with azide](#)

Suzanne Elizabeth Howson

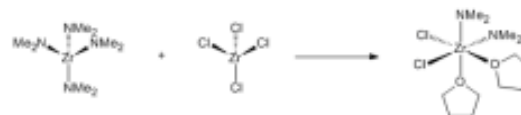
Published: May 06 2010



[Amide/halide metathesis at zirconium](#)

Peter Scott

Published: Mar 19 2010



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The free chemical database

Reaction Database Look-up

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Nucleophilic substitution at benzyl halide with azide; (azidomethyl)benzene

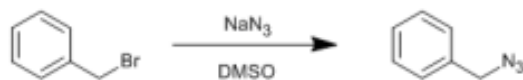
SyntheticPage 408

DOI: [10.1039/SP408](https://doi.org/10.1039/SP408)

Submitted May 06, 2010, published May 06, 2010

Suzanne Elizabeth Howson (s.e.howson@warwick.ac.uk)

A contribution from [Scott group, Warwick University](#)



Chemicals Used

Benzyl bromide

Procedure

Benzyl bromide (2.0 ml, 16.84 mmol, 1.0 eq.) was dissolved in DMSO (40 ml). Sodium azide (1.64 g, 25.26 mmol, 1.5 eq.) was added as a solid and the reaction mixture was stirred overnight at ambient temperature. Water (75 ml) was added *slowly* (exothermic) before extracting the product into diethyl ether (3 × 150 ml). The combined diethyl ether layers were washed with brine (2 × 150 ml), dried over sodium sulfate and the solvent removed to leave a clear oil which was sufficiently pure for use in further reactions (see uploaded NMR spectra) and gave a reasonable combustion analysis. Yield = 1.63 g, 12.24 mmol, 73%.

Author's Comments

Organic azides are energy-rich molecules and there is a risk of explosion. You should perform a risk assessment. See also Kolb, H.C., Finn, M.G., Sharpless, K.B. [Angew. Chem. Int. Ed., 2001, 40, 2004-2021.](#)

Data

¹H NMR (400 MHz, 298 K, CDCl₃) 7.42-7.32 (5H, m, Ph), 4.35 (2H, s, CH₂).

“App-Based Spectroscopy”

- What could be possible for spectra?
 - Process
 - View
 - Predict
 - Analyse

“App-Based Spectroscopy”

- What could be possible for spectra?
 - Process
 - View
 - Predict
 - Analyse
- Already available
 - Do we need to process?
 - View
 - Predict
 - Analyse

Spectra online

▼ Spectra

[Edit](#)

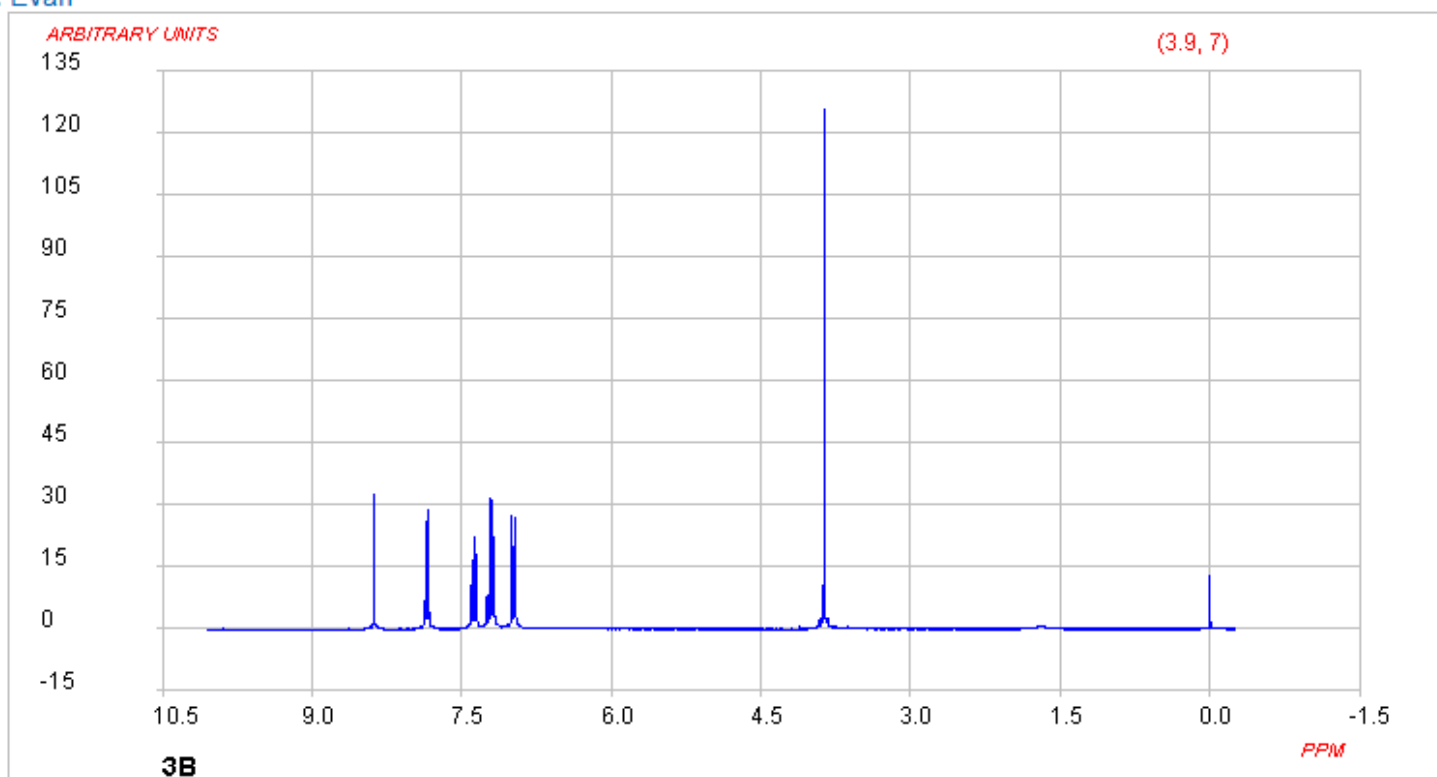
• Type: HNMR

Associated Hyperlink: <http://usefulchem.wikispaces.com/Exp269>

Comments: NMR solvent CDCl₃, 300MHz varian. Bradley Lab, Drexel University, Philadelphia, PA.

Approved: No

Submitted by: [Evan](#)

[OPEN DATA](#)[Download](#)

JSpecView

<http://jspecview.sourceforge.net/>

- Open Source Java applet from Bob Lancashire
- Supports display of JCAMP format spectra
- Used on ChemSpider and supported in browsers with **Java** support

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- Used on ChemSpider and supported in browsers with **Java** support

Does the iPad support Java?

No. iPhone OS 3.2 will not support Java. The iPhone does not support Java. Steve Jobs has been quoted as saying "Java's not worth building in. Nobody uses Java anymore. It's this big heavyweight ball and chain."

Java fans should not expect Apple to reverse this long-standing decision on the iPad.

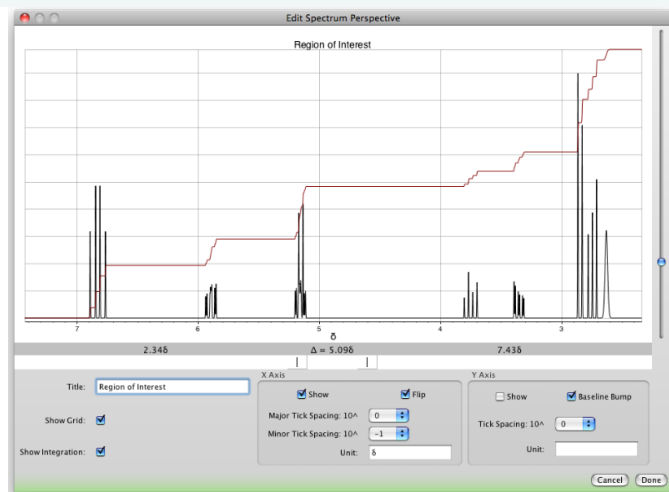
Web Components

- An **open-source and free** HTML5 toolkit.
- For desktop and mobile browsers.

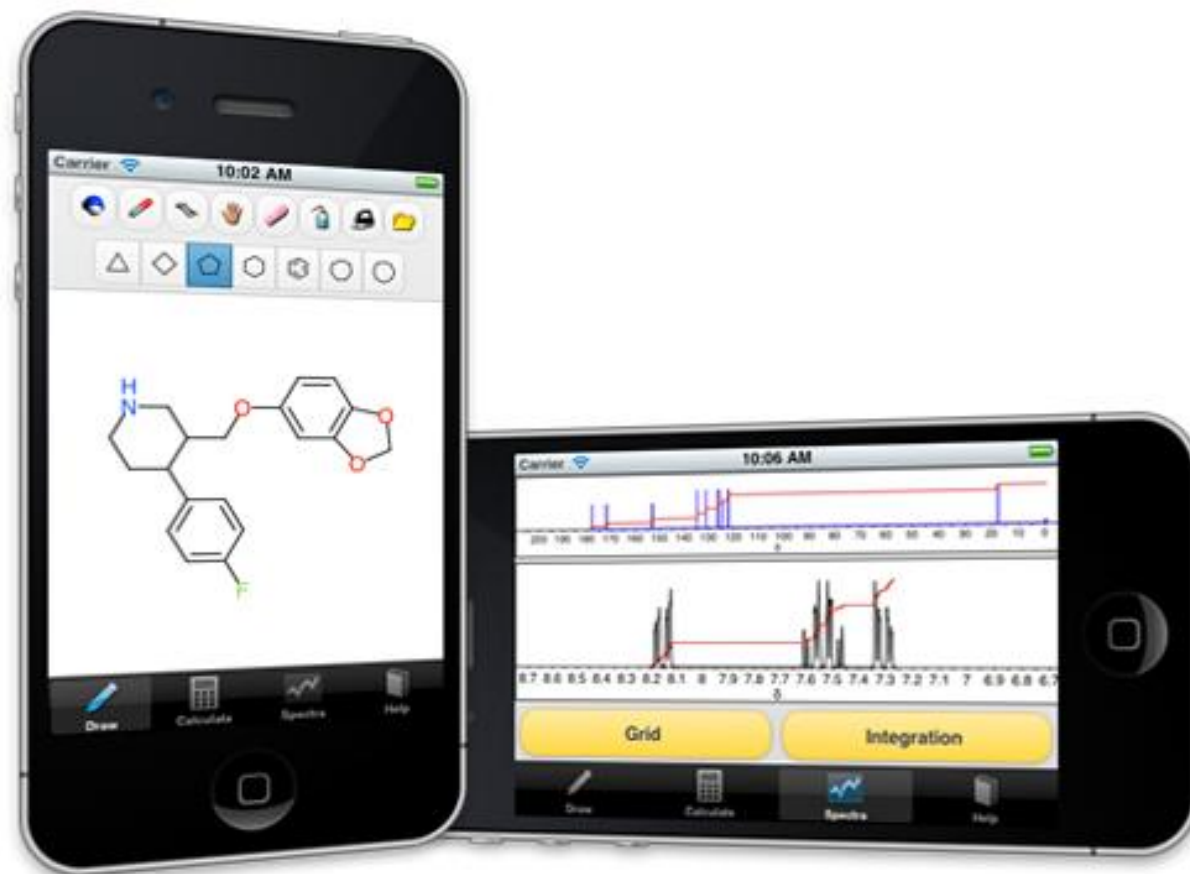


JCAMP-DX Format

ChemDoodle reads mass spectrometry, nuclear magnetic resonance spectroscopy, infrared spectroscopy and other spectra from JCAMP-DX files.



Spectra in the hand



Sourcing information about SciApps

<http://www.scimobileapps.com/>

- An increasing number of Science Apps
- Different platforms, different versions
- How do you track them? Search them?
- Where can developers post information about their apps?
- iTunes does not segregate based on science
- Introducing the [SciMobileApps Wiki...](#)





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Main Page

1 open e-mail-confirmed [account request](#) pending

Navigation

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- [5 Publications and Presentations](#)
- [6 App of the Month](#)
- [7 What Apps are Missing?](#)

[\[edit\]](#) **The Vision for the SciMobileApps Wiki**

Mobile apps for science are expanding in scope and capability very quickly, yet there is no easy way to source information regarding what is available, what the community thinks of these apps (in terms of general reviews) and clustering of these apps into functional groupings. That is the intention of this wiki. It is a community resource for developers and users to share information about the various science apps that are available. We encourage you to participate by adding your comments and adding new pages!

[\[edit\]](#) **The Hosts of SciMobileApps**

SciMobileApps is hosted for the community by two scientists interested in how Mobile Apps can contribute to the worlds of chemistry and Drug Discovery.

[Antony Williams](#) [↗](#) is a part of the online social network as [ChemConnector](#) [Wikipedia](#) [↗](#) [Twitter](#) [↗](#) [Blog](#) [↗](#) [LinkedIn](#) [↗](#)

[Sean Ekins](#) [↗](#) is a part of the online social network as [CollabChem](#) [Wikipedia](#) [↗](#) [Twitter](#) [↗](#) [Blog](#) [↗](#) [LinkedIn](#) [↗](#)

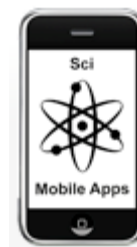
Follow SciMobileApps on Twitter [here](#) [↗](#)

SciMobileApps Wiki

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- 3 Publishers
- 4 Structure Drawing, Visualization and Chemical Databases
- 5 Chemical Calculators
- 6 Chemical Look-Ups
- 7 Chemical Compounds
- 8 Chemical Reactions
- 9 Chemical Safety
- 10 Spectroscopy
- 11 Theoretical Chemistry
- 12 Periodic Tables

SciMobileApps Wiki



ChemSpider Mobile

ChemSpider Mobile is a free iOS app (iPhone, iPod, iPad) for searching the [ChemSpider](#) online chemical database. It provides the ability to search by drawing a chemical structure, or entering a compound name. The app is very straightforward and easy to learn. Search results are shown in a list showing structure and names. Any search result can be examined in more detail by launching the mobile browser and viewing the structure on the ChemSpider web page.

Although the ChemSpider web page is designed to work well on mobile browsers, the mobile app is more convenient to use, and is currently the best way to search by structure from a mobile device. The structure drawing capabilities are provided by the embedded version of the [Mobile Molecular DataSheet](#). The app was built by [Molecular Materials Informatics](#), on behalf of the [Royal Society of Chemistry](#).

Contents

- 1 Technical Details
 - 1.1 Structure page
 - 1.2 Text page
 - 1.3 Results page
- 2 Logistics
 - 2.1 Licensing & Availability
 - 2.2 External links
 - 2.3 User Reviews

ChemSpider Mobile



Company [Royal Society of Chemistry](#)

Key people [\[Dr. Antony J. Williams\]](#),
[Dr. Alex M. Clark](#)

Science [Chemistry](#)

Website <http://chemspider.com>



Why not use Wikipedia???


Mobile Molecular DataSheet

From Wikipedia, the free encyclopedia



A major contributor to this article appears to have a [close connection with its subject](#). It may require [cleanup](#) to comply with Wikipedia's content policies, particularly [neutral point of view](#). Please discuss further on the [talk page](#). *(November 2010)*

The **Mobile Molecular DataSheet** is (MMDS) is a mobile app which provides chemical structure diagram editing, molecular datasheet management and various other productivity tools. Currently it is available for [BlackBerry](#) smartphones and Apple mobile devices ([iPhone](#), [iPod](#) and [iPad](#)).

MMDS is developed by [Molecular Materials Informatics, Inc.](#) , founded by Dr. Alex M. Clark and headquartered in Montréal, Canada.

Changes in Mobile

- “Apps” are originally iOs branded
- And then came Android...

Yes, Amazon's Kindle Fire is a \$199 Android tablet



New BlackBerry phones to support Android?

RIM's PlayBook will run Android apps

Run Android Apps on Your PC with BlueStacks

Tweet to App in 3 Days

<http://www.slideshare.net/ekinssean/green-solvents-app>

Green Solvents: From Idea to App in 3 Days



Sean Ekins, Alex M. Clark and Antony J. Williams

Social Networking to Apps



collabchem Sean Ekins

ACS Holding Back green chem solvent selection behind ACS wall for user details. Concern about context of use -way too conservative IMHO

23 Jun



collabchem Sean Ekins

ACS Green Chem Conf. Solvent selection in discovery influences API solvent use. Green Chem may also be cheaper.

23 Jun



collabchem Sean Ekins

At ACS green chem conf in DC. Pharma needs an App that tells their chemists which are preferred solvents.

23 Jun

Green Solvents

<http://itunes.apple.com/us/app/green-solvents/id446670983>



Bad



Good

Siri *Knows* Chemistry???

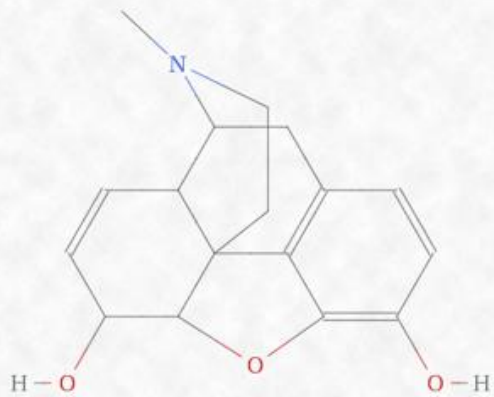
AT&T 9:05 AM

I found this for you:

Input interpretation

morphine structure diagram

Result



WolframAlpha

The image shows a screenshot of an iPhone's Siri interface. At the top, the status bar shows 'AT&T' and '9:05 AM'. Below that, a speech bubble says 'I found this for you:'. Underneath, there's a section for 'Input interpretation' with 'morphine' and 'structure diagram' entered. The 'Result' section displays a chemical structure diagram of morphine, which is a complex polycyclic alkaloid with a pentacyclic ring system, a nitrogen atom, and two hydroxyl groups. The WolframAlpha logo is visible at the bottom of the result area.

WolframAlpha™ computational knowledge engine

Enter what you want to calculate or know about:

morphine

Examples Random

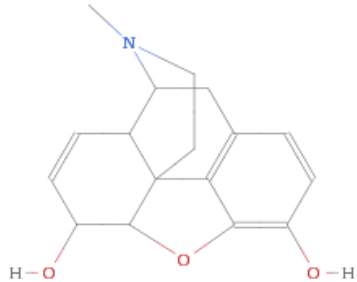
Assuming "morphine" is a chemical compound | Use as a word instead

Input interpretation:
morphine

Chemical names and formulas: [More](#)

formula	$C_{17}H_{19}NO_3$
name	morphine
IUPAC name	(5 α ;6 α ;)–Didehydro–4,5–epoxy–17–methylmorphinan–3,6–diol

Structure diagram: [Show all atoms](#)




The image shows a screenshot of the WolframAlpha website. At the top, the WolframAlpha logo is displayed. Below it, there's a search bar with 'morphine' entered. The results section shows 'Assuming "morphine" is a chemical compound | Use as a word instead'. Underneath, there's a section for 'Input interpretation:' with 'morphine'. The 'Chemical names and formulas:' section contains a table with the following information:

formula	$C_{17}H_{19}NO_3$
name	morphine
IUPAC name	(5 α ;6 α ;)–Didehydro–4,5–epoxy–17–methylmorphinan–3,6–diol

Below this, the 'Structure diagram:' section shows a chemical structure diagram of morphine, identical to the one in the Siri screenshot. A 'Show all atoms' link is visible next to the diagram.

Siri Accesses Information

 **WolframAlpha**™ computational knowledge engine

Enter what you want to calculate or know about:

[Examples](#) [Random](#)

terminal dimethyl



chemical formula, density, melting point, boiling point, ... [Cached page](#) [Refresh](#)

Input interpretation:
terminal dimethyl

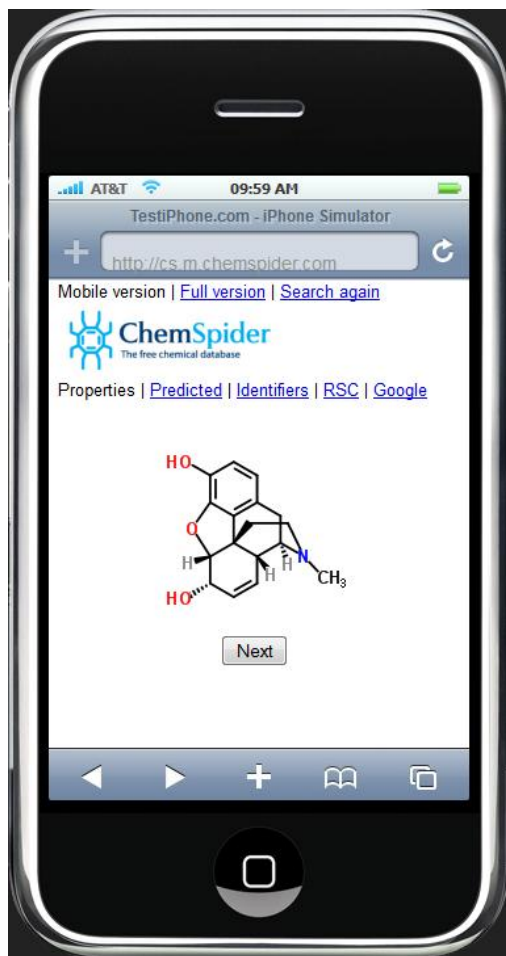
Chemical names and formulas: [More](#)

formula	C_2H_8
name	terminal dimethyl
IUPAC name	methane

Structure diagram: [Show all atoms](#) [Show graph properties](#)



Chemists Know Chemistry



Mobile version | [Full version](#) | [Search again](#)



Properties | [Predicted](#) | [Identifiers](#) | [RSC](#) | [Google](#)



Property	Value
ChemSpider ID	4450907
Molecular Formula	C ₁₇ H ₁₉ NO ₃
Molecular Weight	285.3377
Nominal Mass	285 Da
Average Mass	285.338 Da
Monoisotopic Mass	285.137 Da
Systematic Name	
InChIKey	BQJCRHHNABKAKU-KBQPJGBKBH

Conclusions

- More mobile adoption is inevitable – mobile is simply “smaller computers”
- The discrimination of Apps will be based on:
 - Ease of use
 - Quality of prediction algorithms
 - Access to quality content
- Running list of Chemistry Apps is updated here:
<http://www.slideshare.net/AntonyWilliams/>

Smart Phones

JOURNAL OF
CHEMICAL EDUCATION

COMMENTARY

pubs.acs.org/jchemeduc

Smart Phones, a Powerful Tool in the Chemistry Classroom

Antony J. Williams^{*,†} and Harry E. Pence[‡]

[†]ChemSpider, Royal Society of Chemistry, U.S. Office, Wake Forest, North Carolina 27587, United States

[‡]Department of Chemistry and Biochemistry, SUNY College at Oneonta, Oneonta, New York 13820, United States

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Chemical Sciences

 **ChemSpider**
The free chemical database

In Press



Smartphones and tablet computers can now be used to perform many of the operations previously addressed by laptops or desktop computers and they represent an exciting new computing platform for drug discovery, particularly in chemistry.

Mobile apps for chemistry in the world of drug discovery

**Antony J. Williams¹, Sean Ekins², Alex M. Clark³,
J. James Jack⁴ and Richard L. Apodaca⁵**

¹ Royal Society of Chemistry, 904 Tamaras Circle, Wake Forest, NC 27587, USA

² Collaborations in Chemistry, 601 Runnymede Avenue, Jenkintown, PA 19046, USA

³ Molecular Materials Informatics, 1900 St. Jacques #302, Montreal, Quebec, Canada H3J 2S1

⁴ Accelrys Ltd. (formerly Symyx UK Ltd), 334 Cambridge Science Park, Cambridge CB4 0WN, UK

⁵ Metamolecular, LLC, 8070 La Jolla Shores Drive #464, La Jolla, CA 92037, USA

Mobile hardware and software technology continues to evolve very rapidly and presents drug discovery scientists with new platforms for accessing data and performing data analysis. Smartphones and tablet computers can now be used to perform many of the operations previously addressed by laptops or desktop computers. Although the smaller screen sizes and requirements for touch-screen manipulation can present user-

Antony J. Williams graduated with a PhD in chemistry as an NMR spectroscopist. He is currently Vice President, Strategic Development for ChemSpider at the Royal Society of Chemistry. Antony has written chapters for many books and authored or peer reviewed more than 120 papers and book chapters on NMR, predictive absorption, distribution, metabolism and excretion (ADME) methods, Internet-based tools, crowd-sourcing and database curation. He is an active blogger and participant in the Internet chemistry network.



Sean Ekins graduated from the University of Aberdeen, receiving his MSc, PhD and DSc. He is Principal Consultant for Collaborations in Chemistry and Collaborations Director at Collaborative Drug Discovery Inc. He has written over 170 papers and book chapters on topics including drug metabolism, drug-drug interaction screening, computational ADME/Tox, collaborative computational technologies and neglected disease research. He



There's an "App for That"

\$0.99



DAVANDER MOBILE



CatPaint

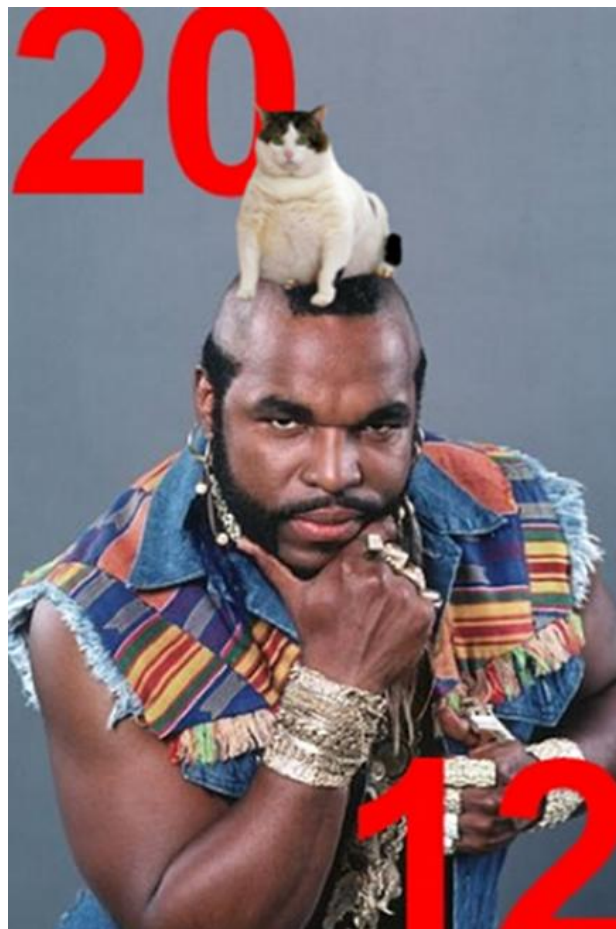
Add cats to any photo.

The premier cat-based image editor for the iPhone and iPod Touch.

Effortlessly add any of sixteen adorable cats to your photos using an intuitive gesture interface. New in version 2.0 cats come equipped with lasers, for inter-galactic kitty-combat!

Available on the
App Store

There's an "App for That"



Thank you

Email: williamsa@rsc.org

Twitter: ChemConnector

Blog: www.chemspider.com/blog

Personal Blog: www.chemconnector.com

SLIDES: www.slideshare.net/AntonyWilliams

