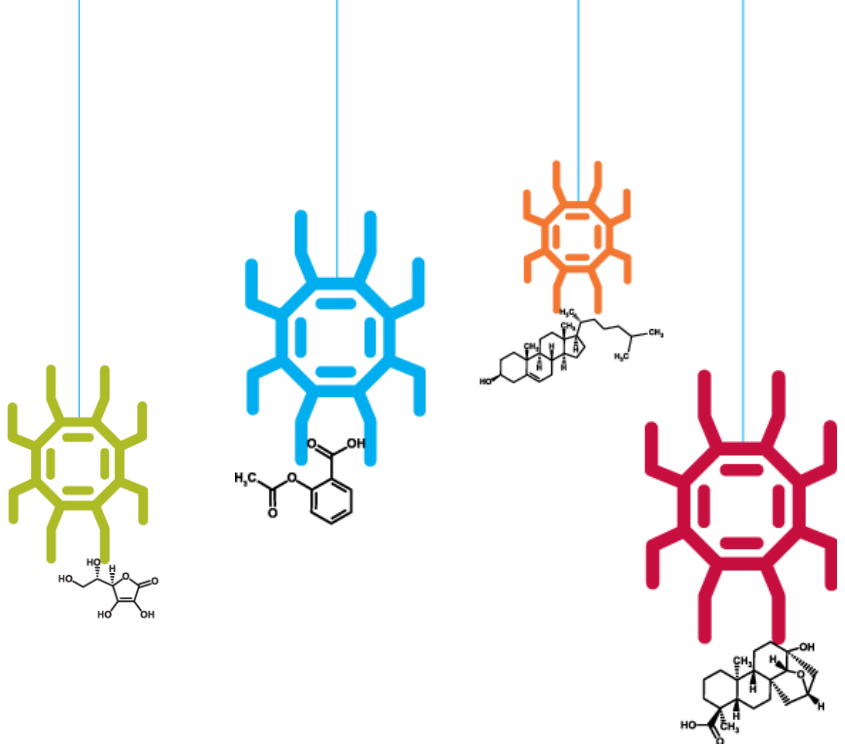

Mobile devices and “Generation App”

Antony Williams

ICIC Conference

October 2011

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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..

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The free chemical database

There's an "App for That"

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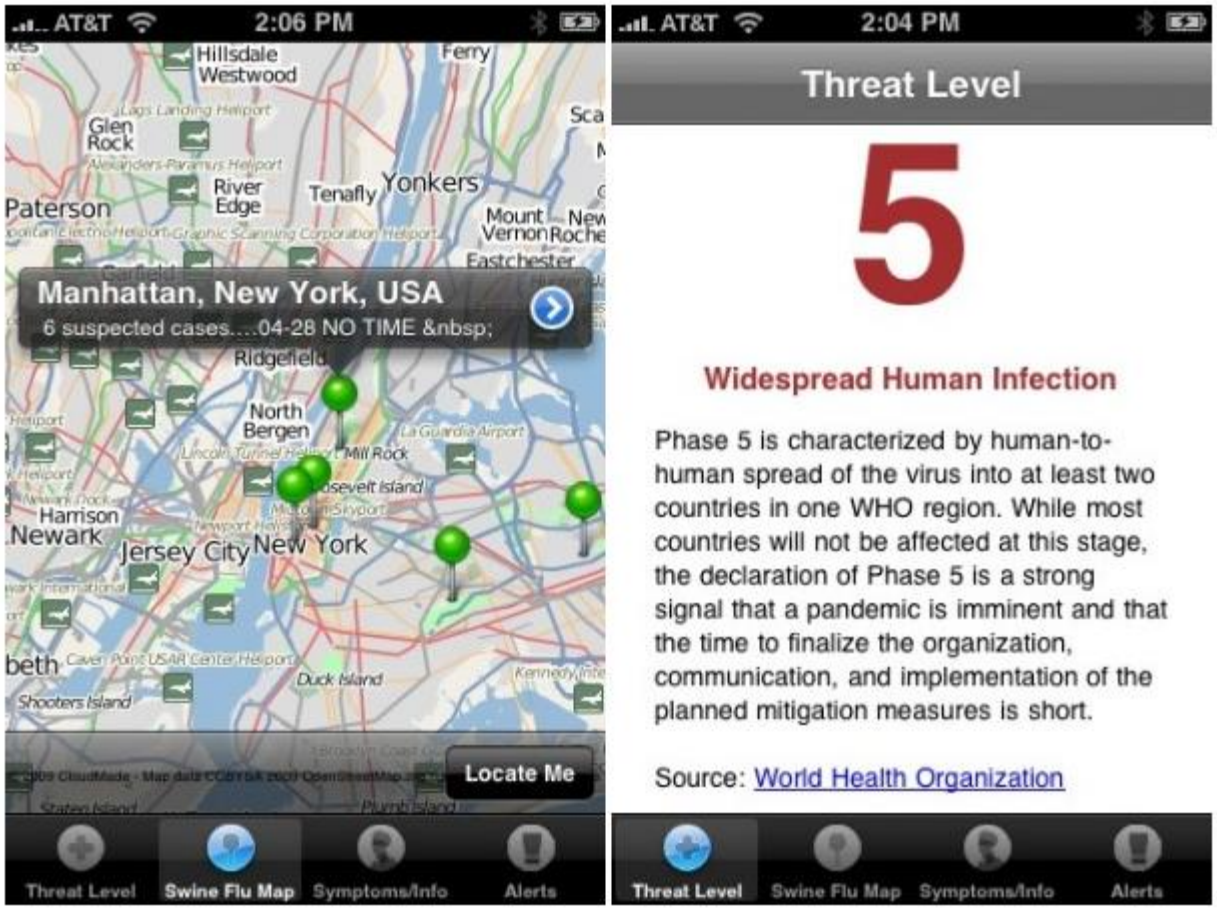
There's an "App for That"



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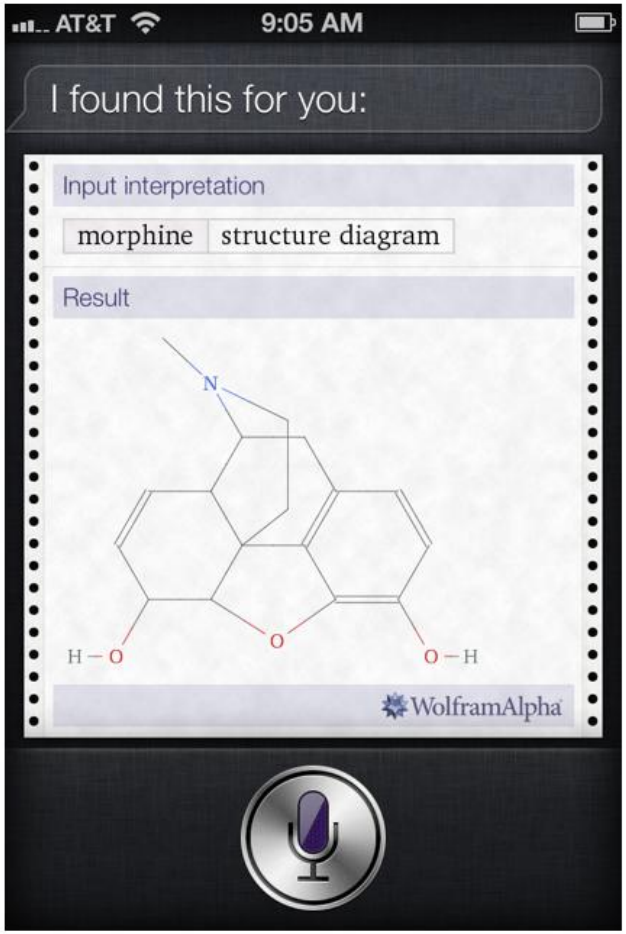
Siri Knows Chemistry



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There's a lot of Mobile Chemistry!

- Categorization of chemistry apps. More later…

Contents

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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

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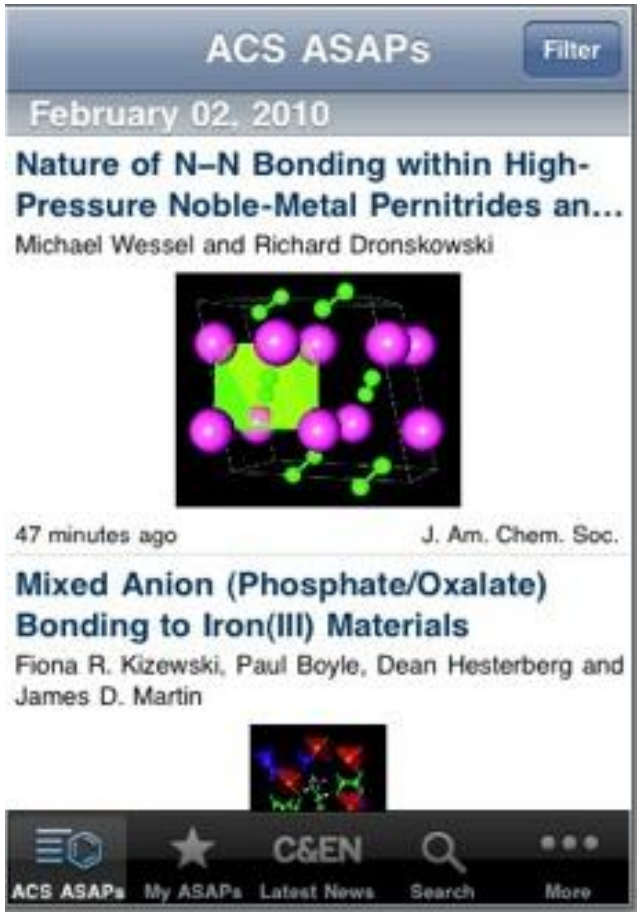
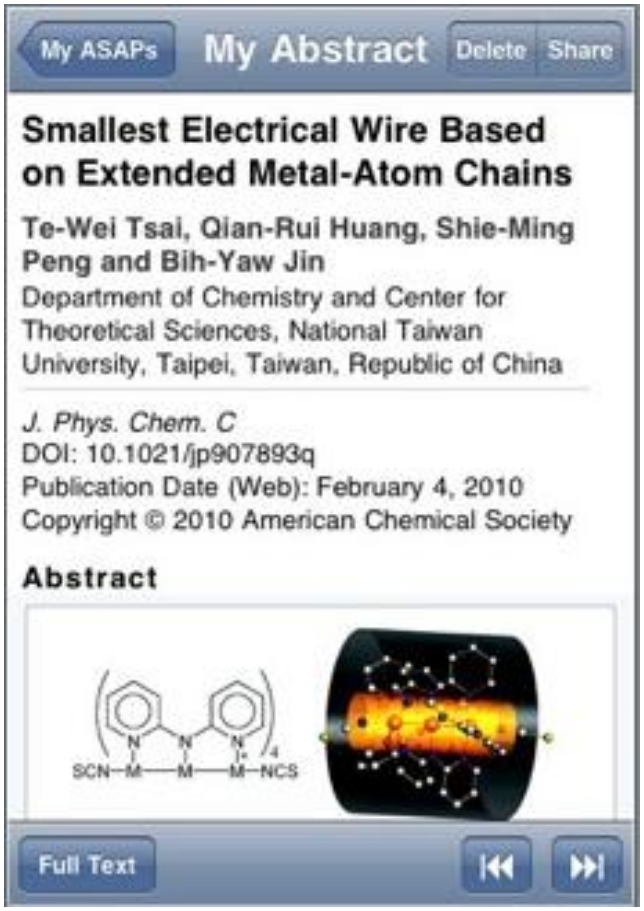
Scientific Publisher Apps (ACS)

http://tinyurl.com/ykaprhf





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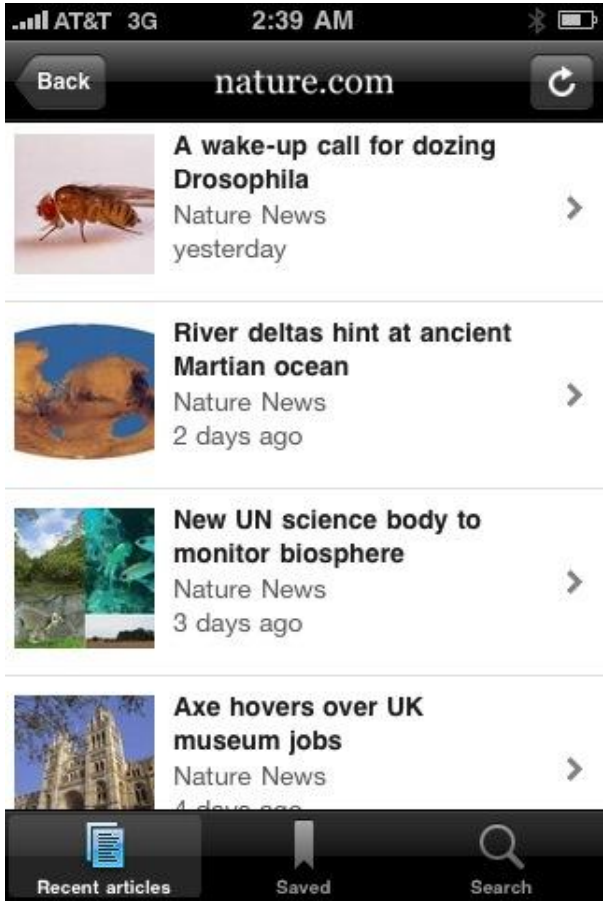
Scientific Publisher Apps (Nature)

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



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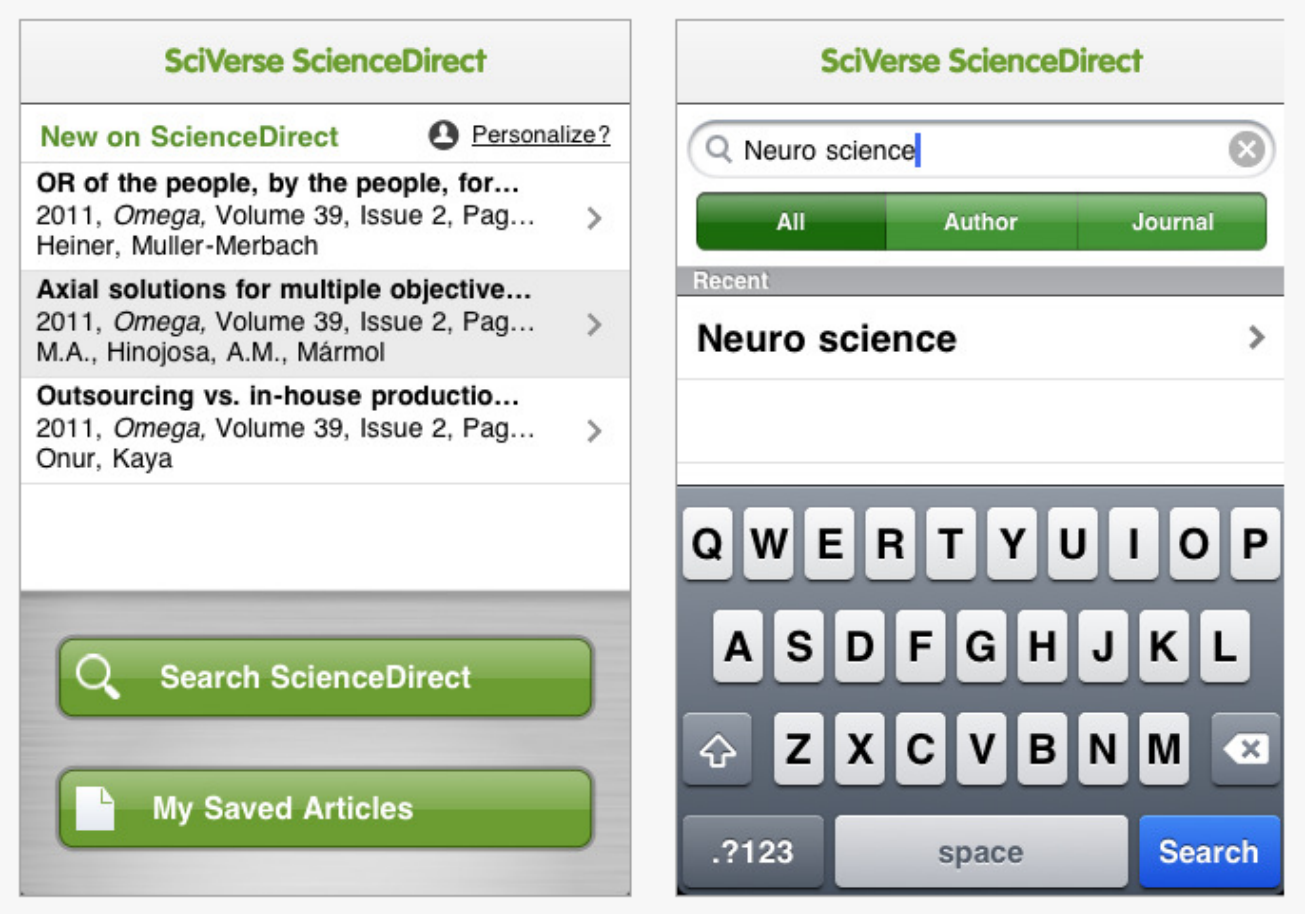
SciVerse ScienceDirect

http://tinyurl.com/3czq37y



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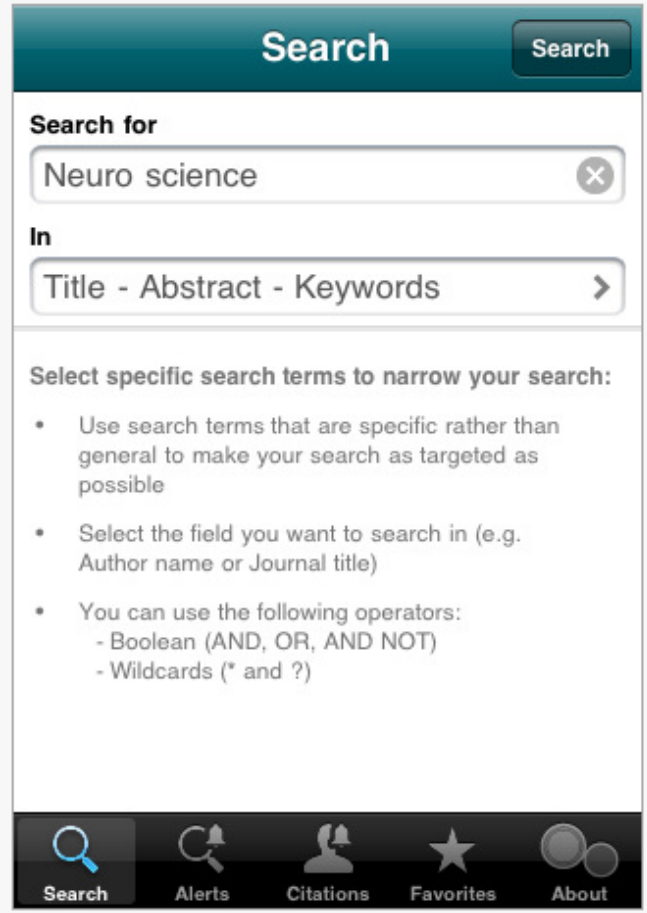
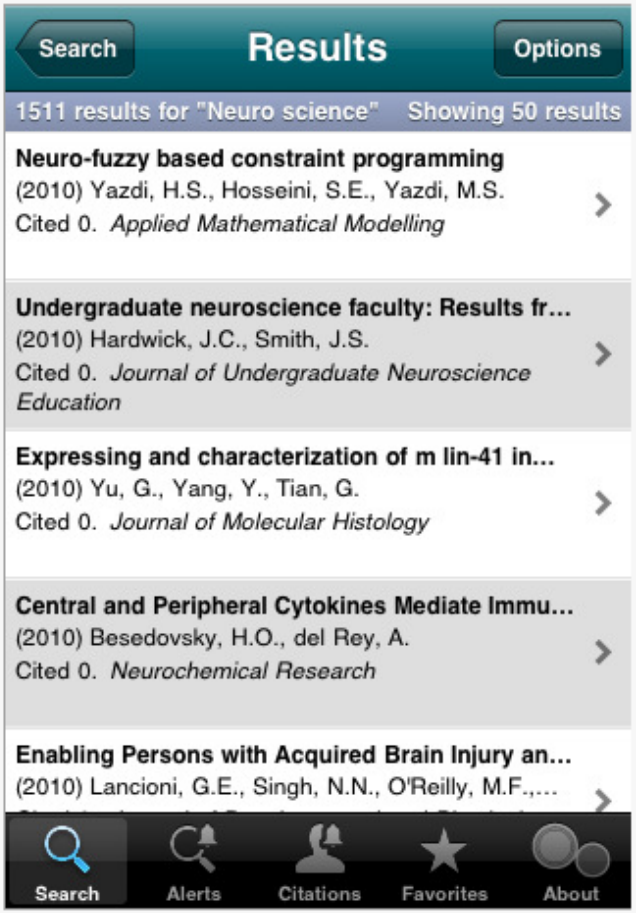
Sciverse Scopus

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





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Science App

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

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Online Tools for Publications

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ONS Open Melting Point Collection JC Bradley, ASID Lang, AJ Williams, E Curtin Nature Publishing Group		2011
A quality alert and call for improved curation of public chemistry databases AJ Williams, S Ekins Drug Discovery Today		2011

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“Papers” for Managing Publications

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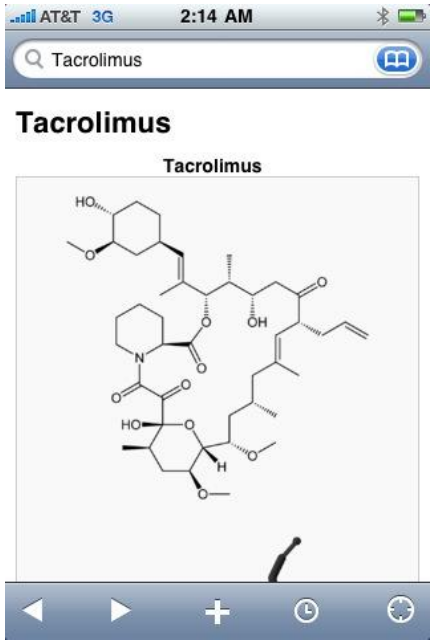
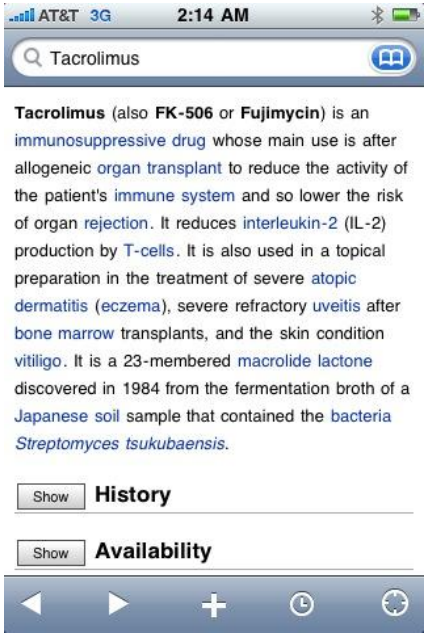
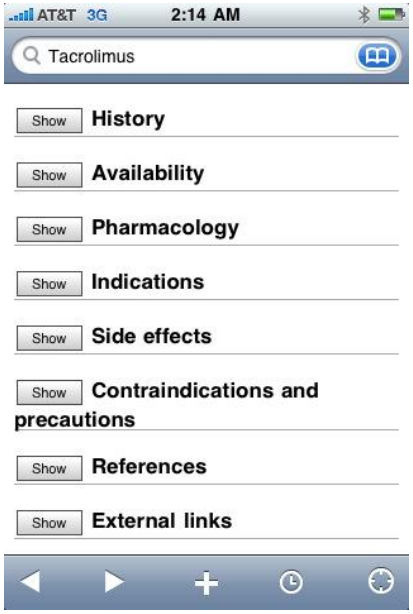
Wikipedia Chemistry







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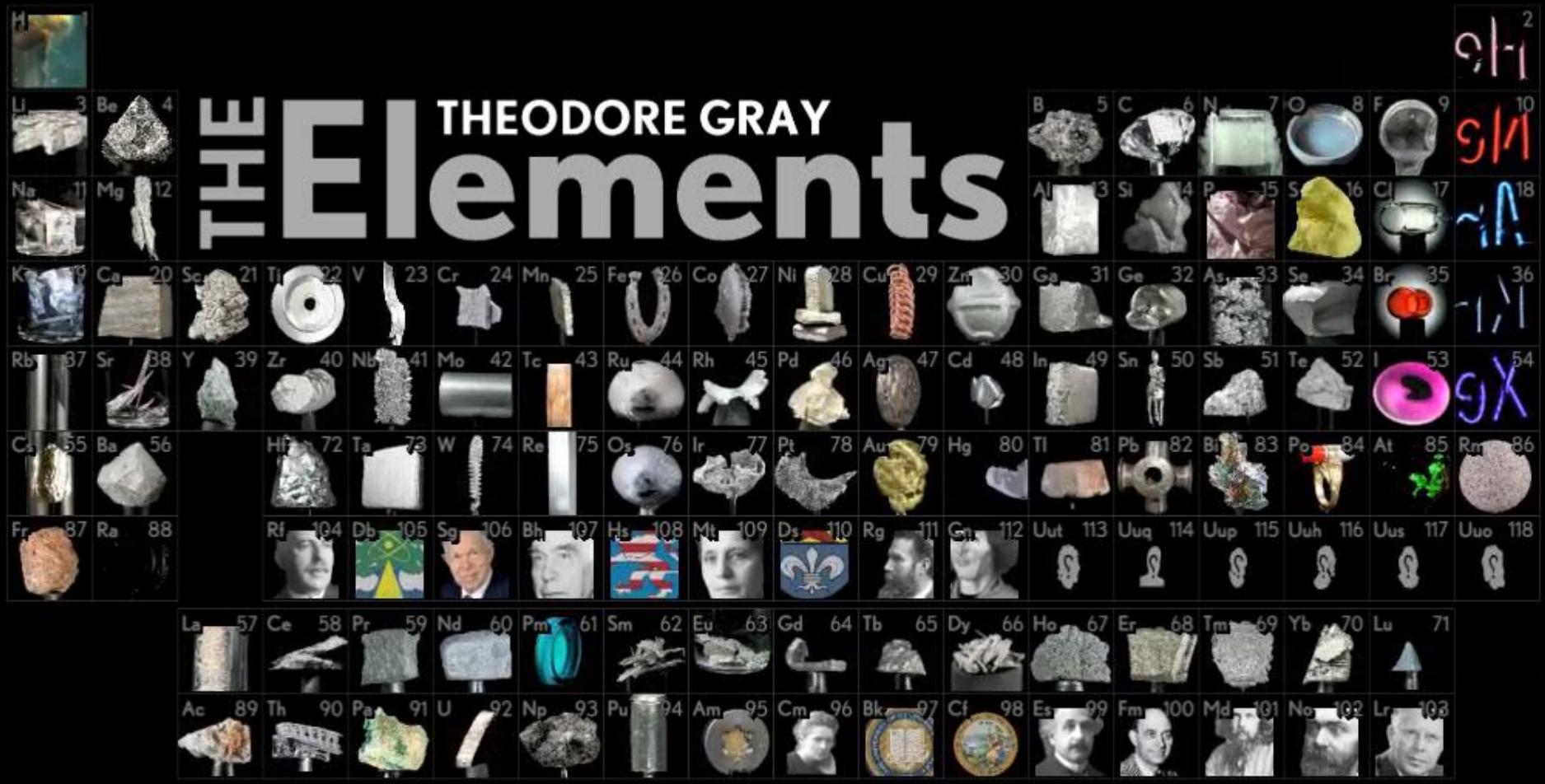
search

THE Elements

THEODORE GRAY



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.

PHOTOGRAPHS BY THEODORE GRAY AND NICK MANN

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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).

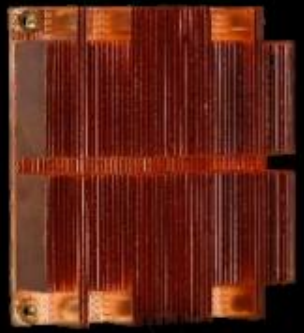
Unbeknownst to the ancients, copper has another nice attribute: the second-highest electrical conductivity of any metal. Vast quantities of copper are used for electrical wiring, making it as vital to the modern age as it was to the Bronze Age.

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 electrowinning nodule.



Solid copper heat sink for a CPU chip.

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

Copper electrical cable thick enough to carry 400 amps.

Coppersmiths make cups and pitchers by hand from copper sheet.

Cu 29

Copper

Atomic Radius
145pm

Crystal Structure
Face Centered Cubic

Electron Shells
$[Ar]3d^{10}4s^{1}$

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

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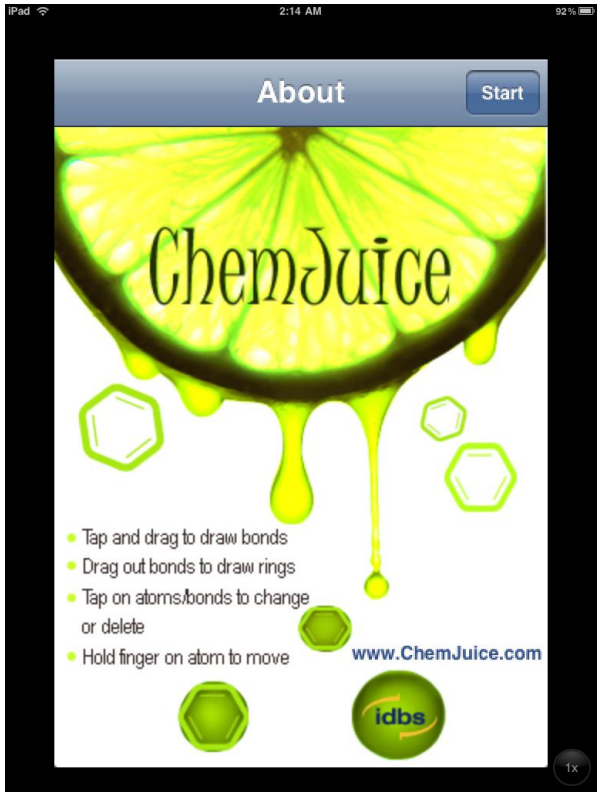
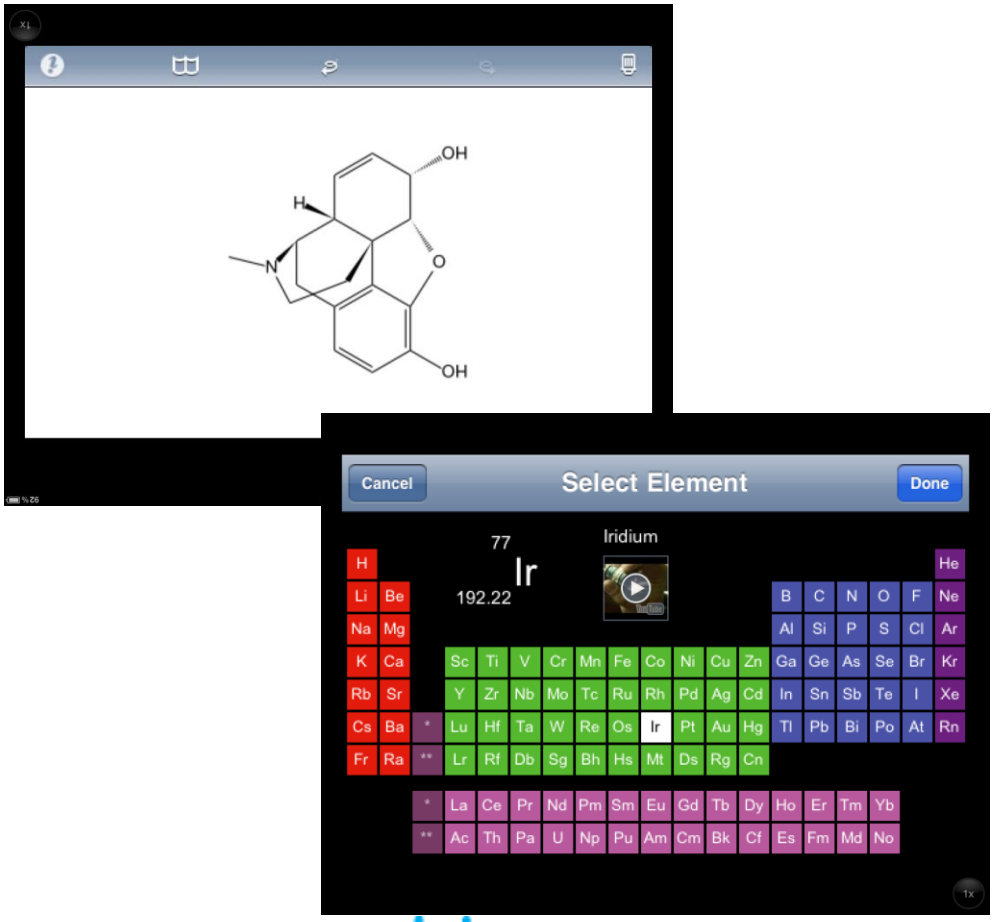
Structure Drawing as an entry point

- 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





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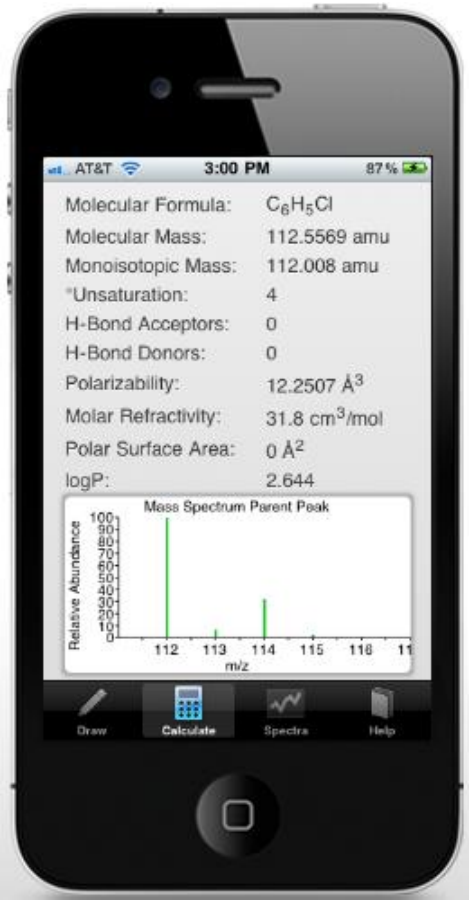
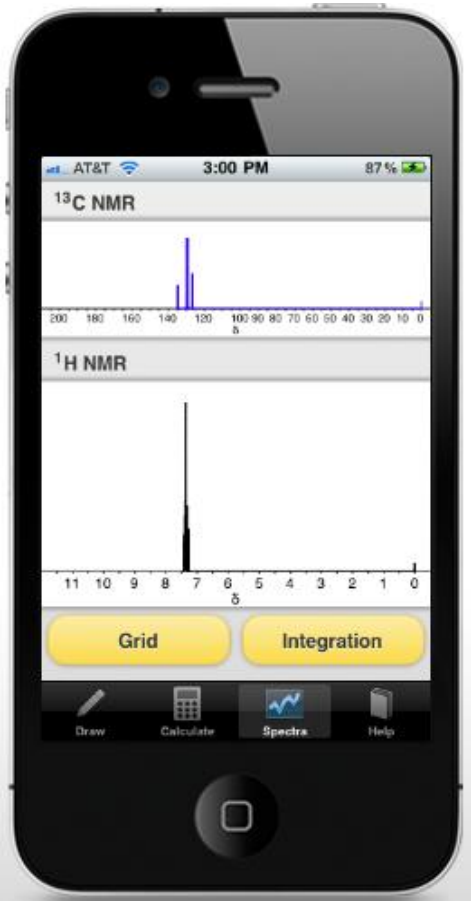
ChemDoodle Mobile





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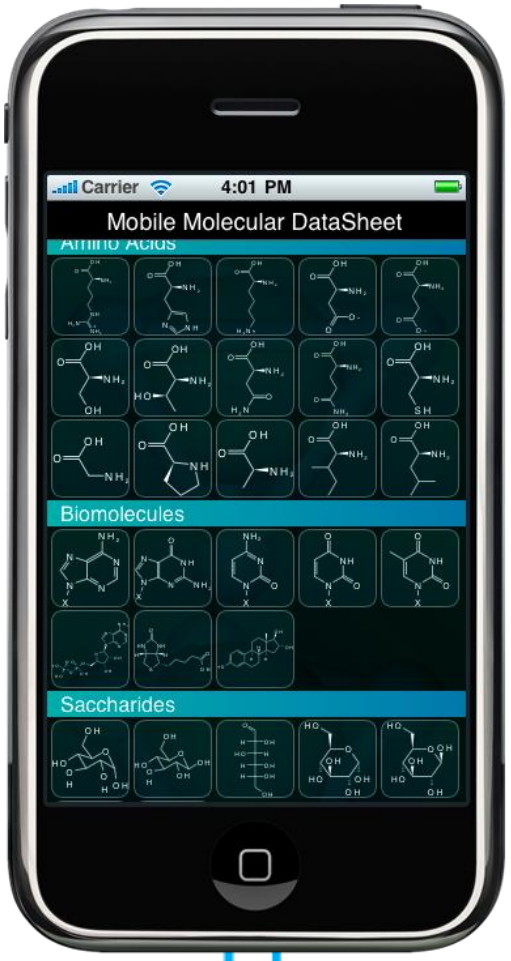
Chemical Structure Drawing Mobile Molecular Datasheet



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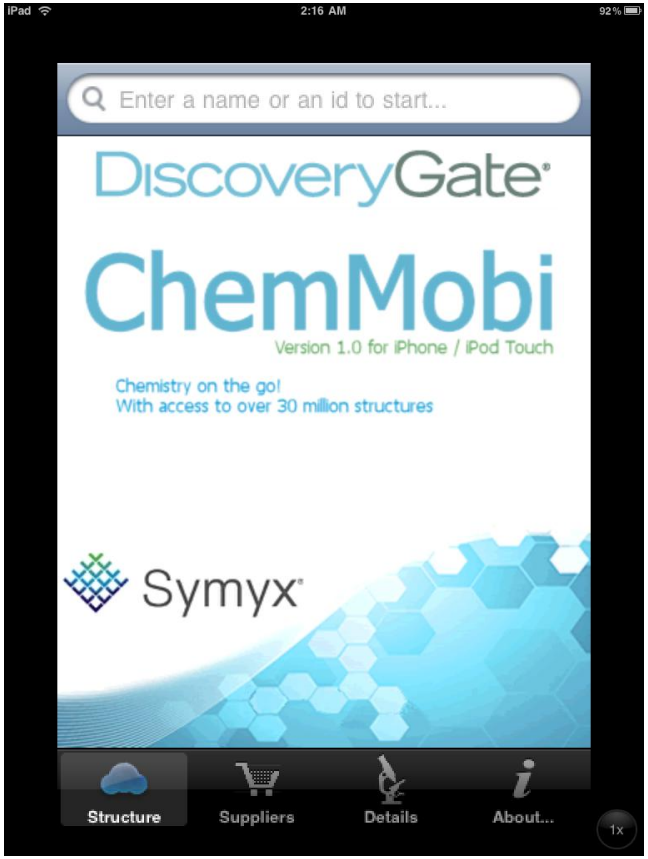

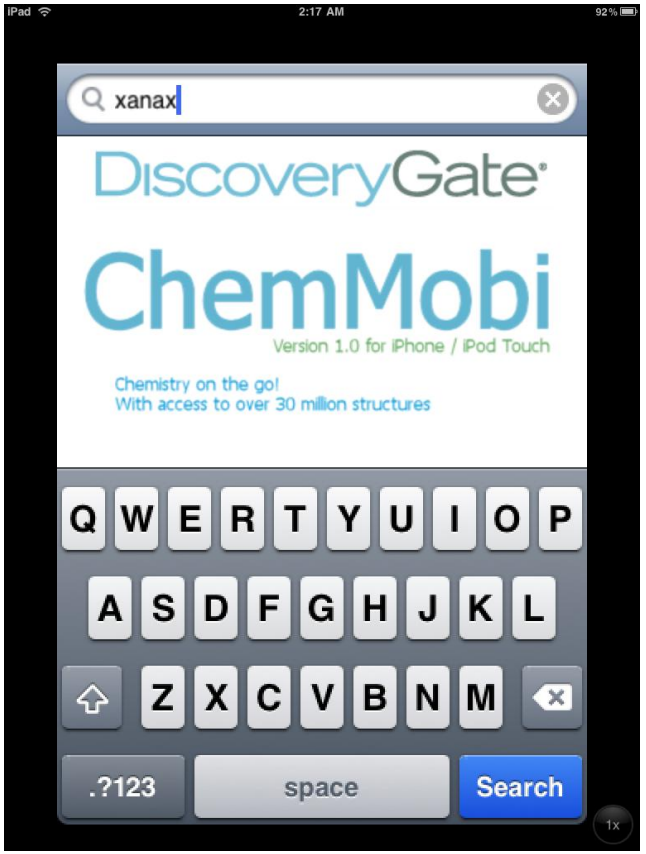

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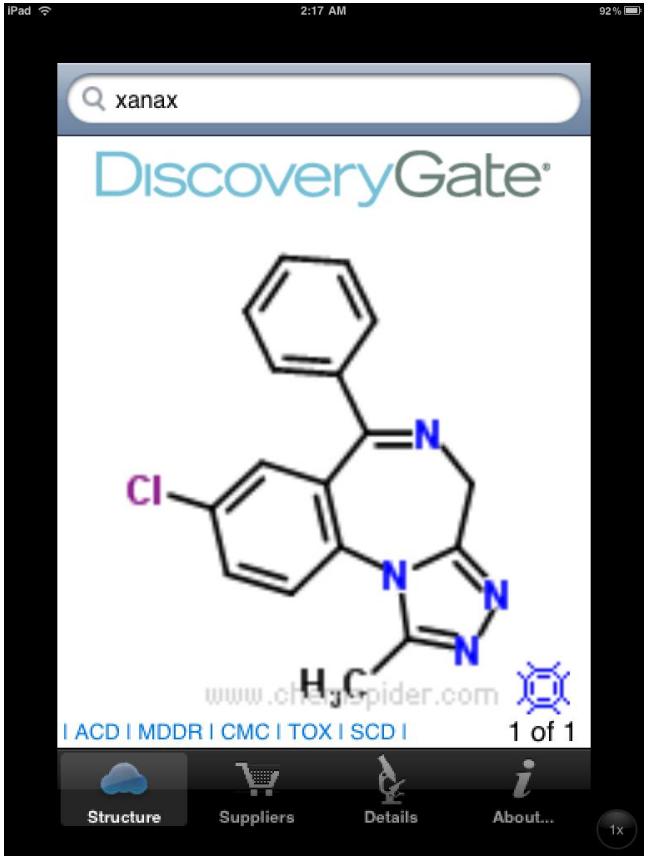

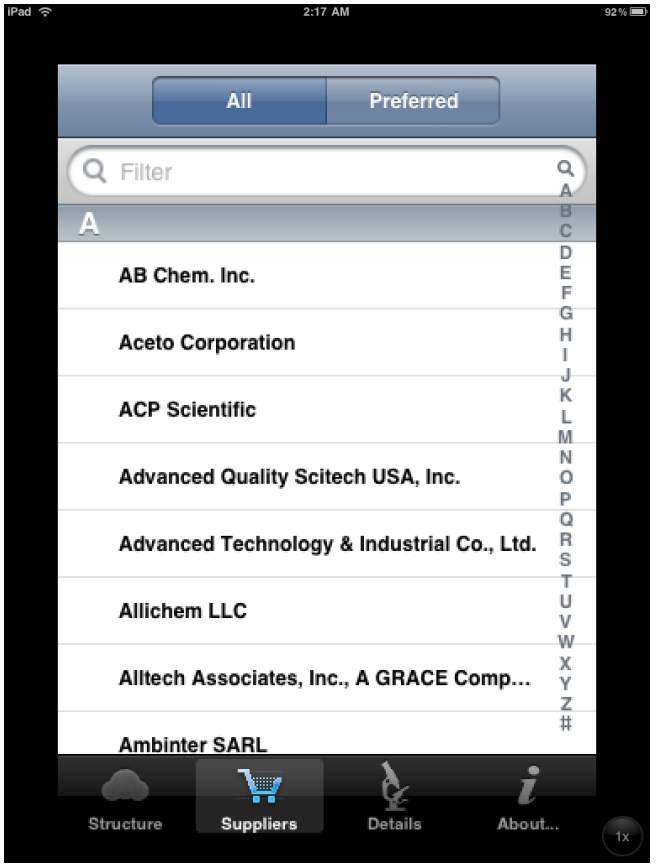

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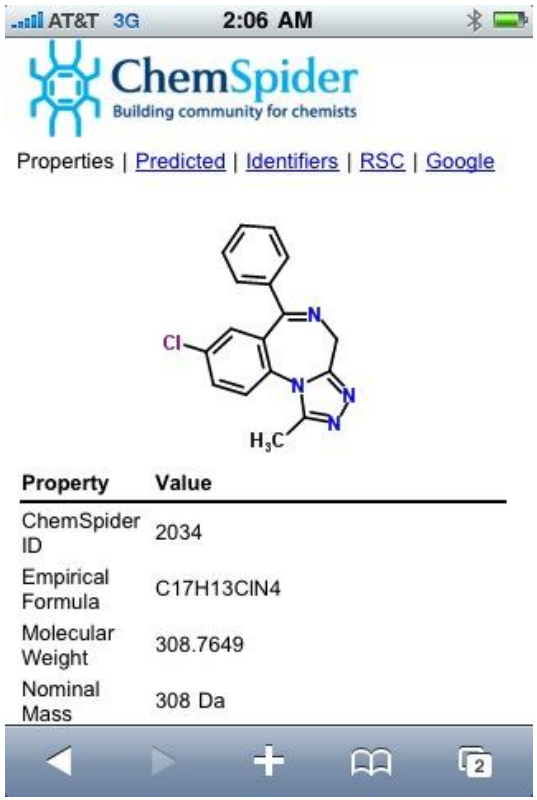

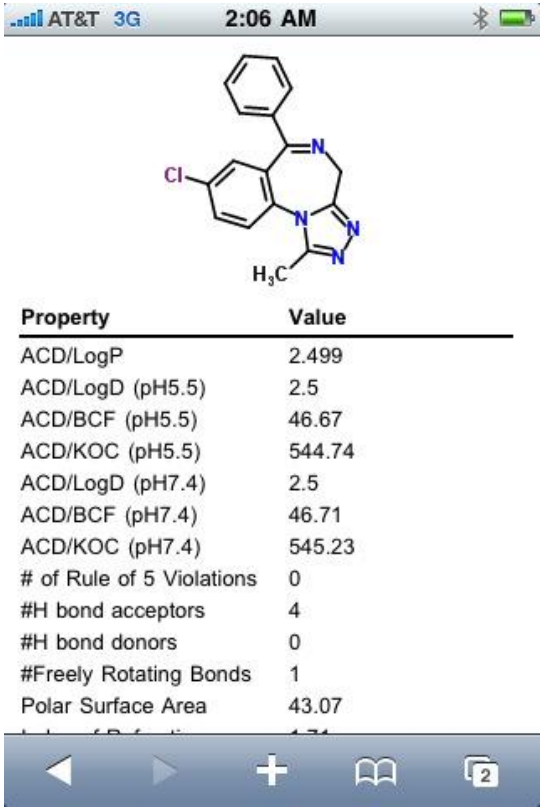

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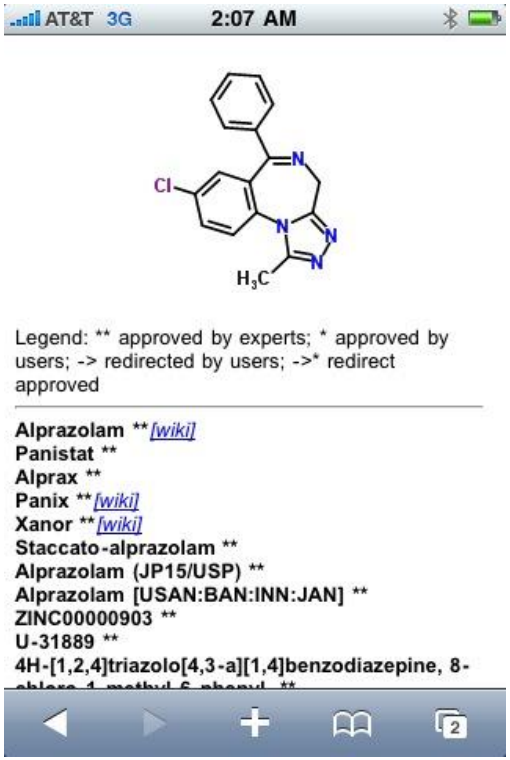

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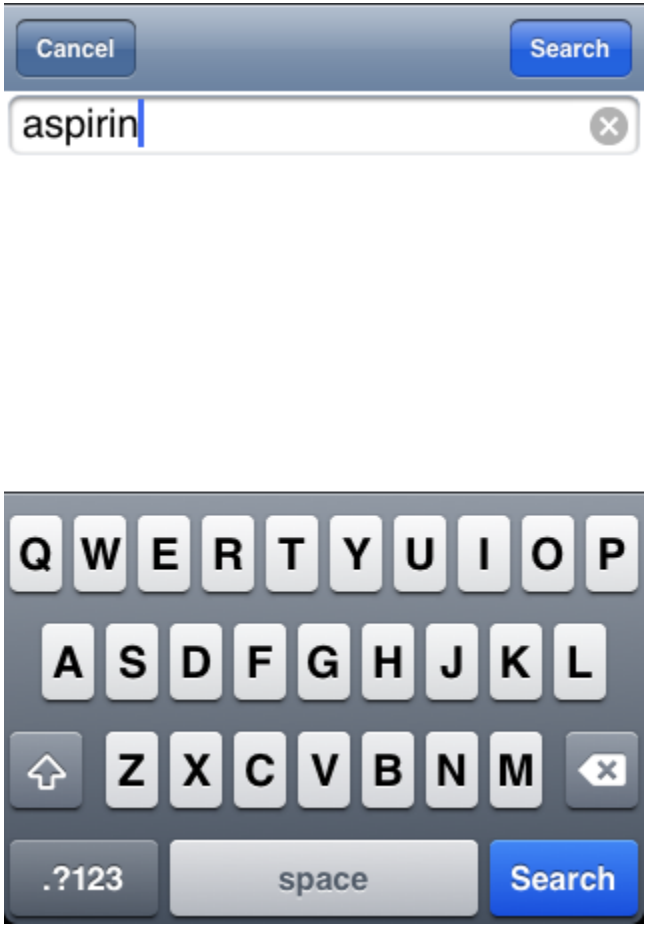
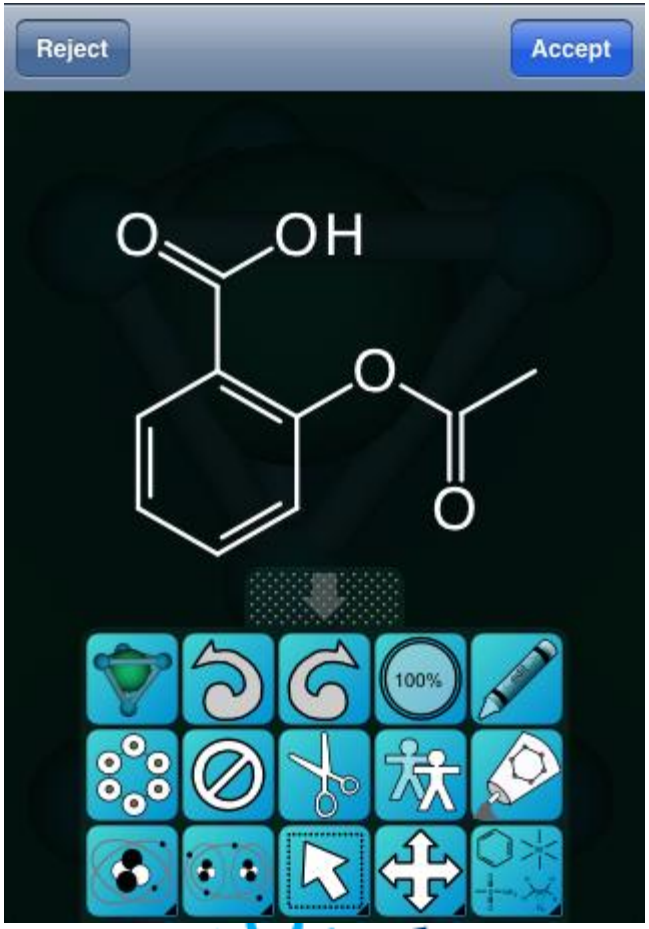
Text and Structure Searching





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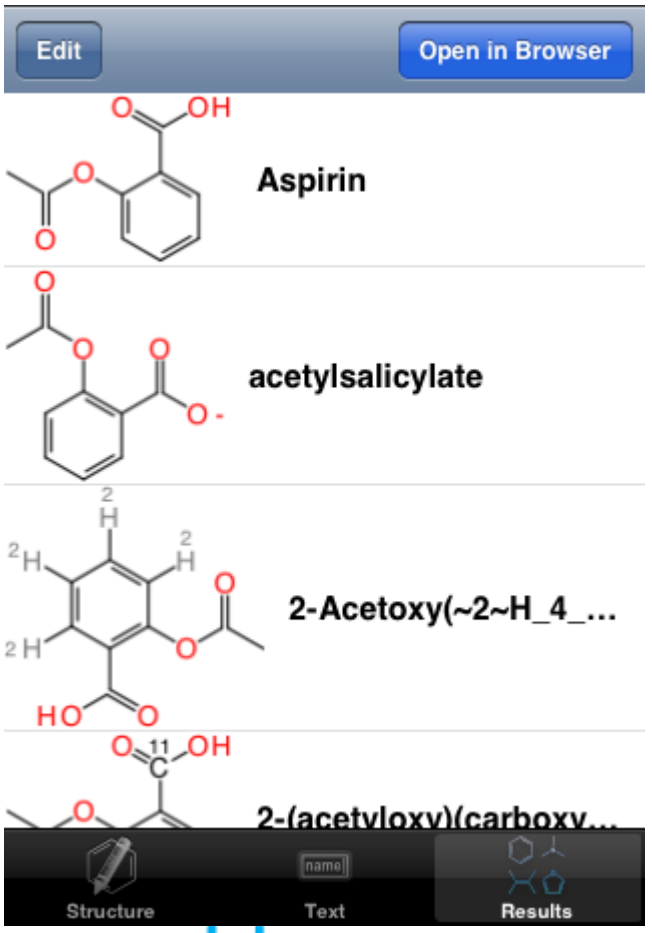
Exact and Skeleton Search



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Open in Browser

- Coming soon:
  - Substructure searching
  - Similarity searching

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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

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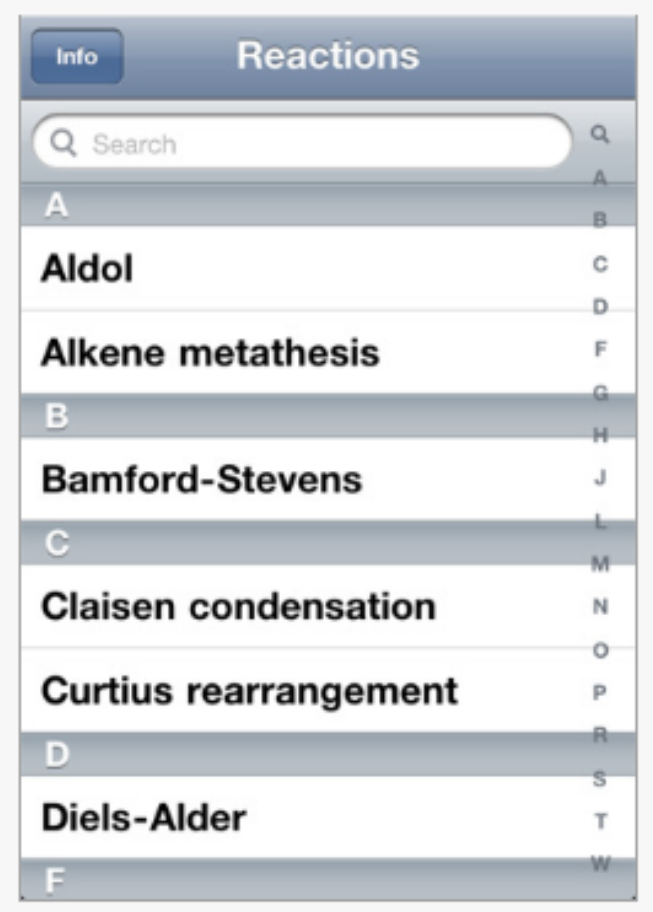
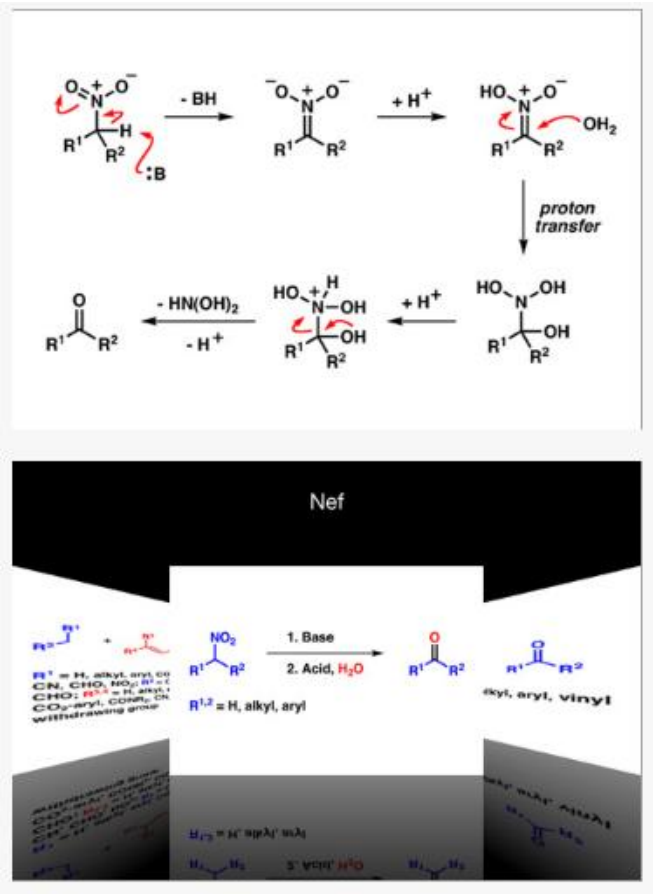
Named Reactions

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





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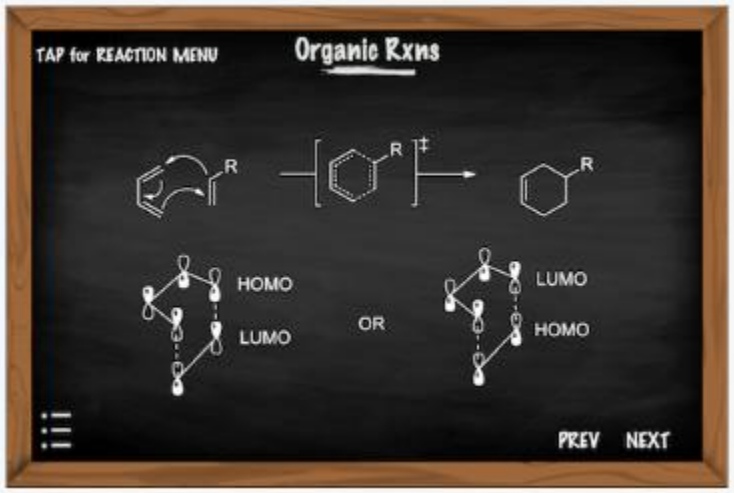
Organic Named Reactions

http://tinyurl.com/3d54fvv



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ReactionFlash

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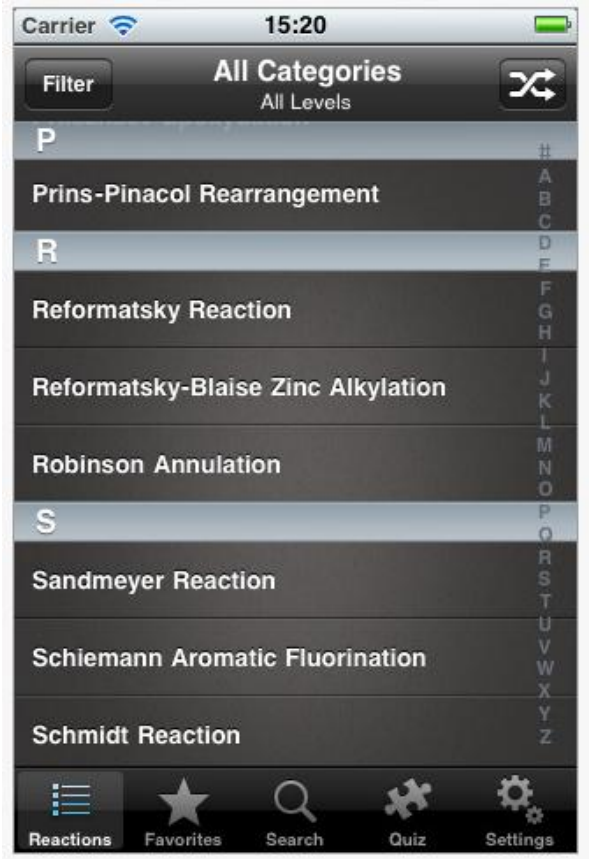

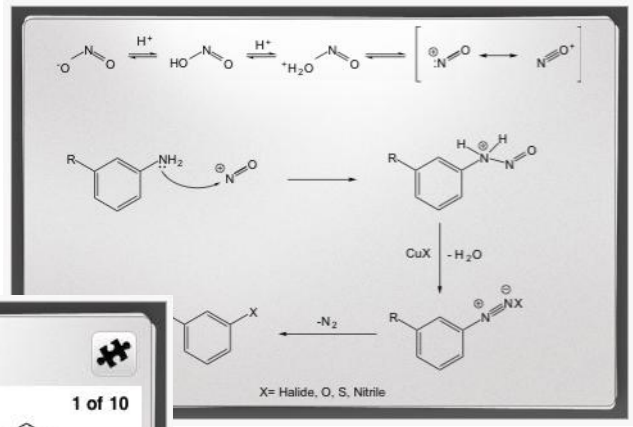

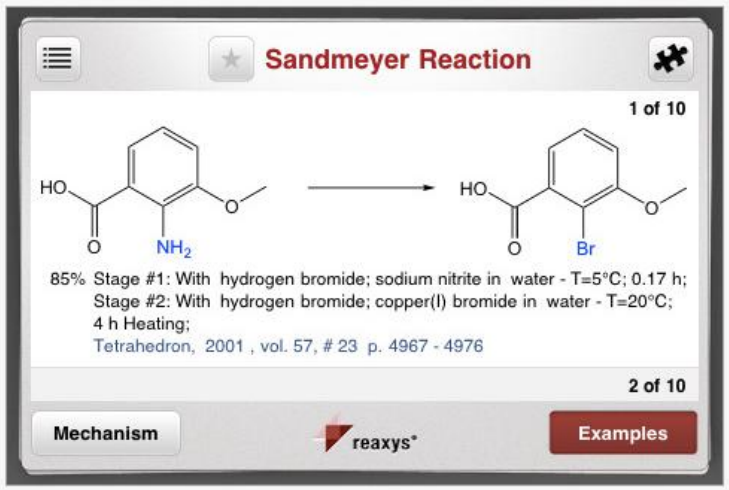

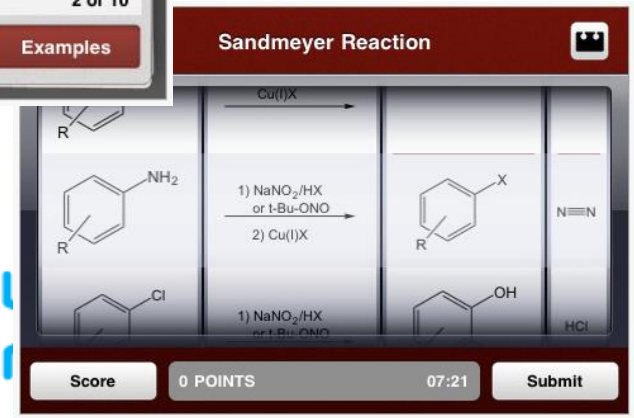

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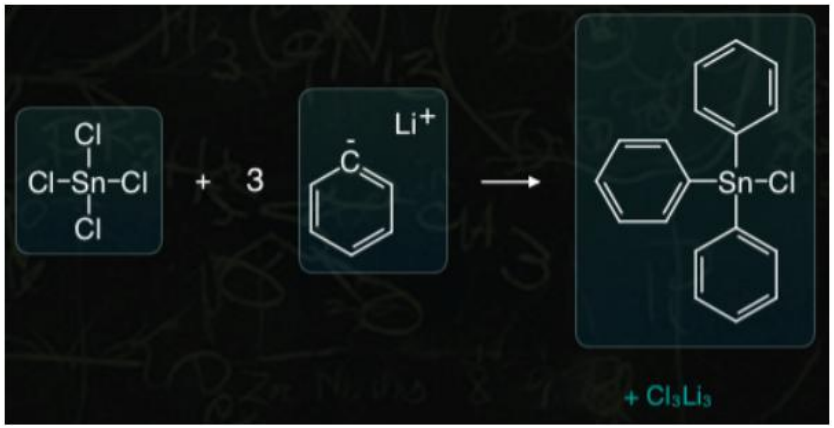
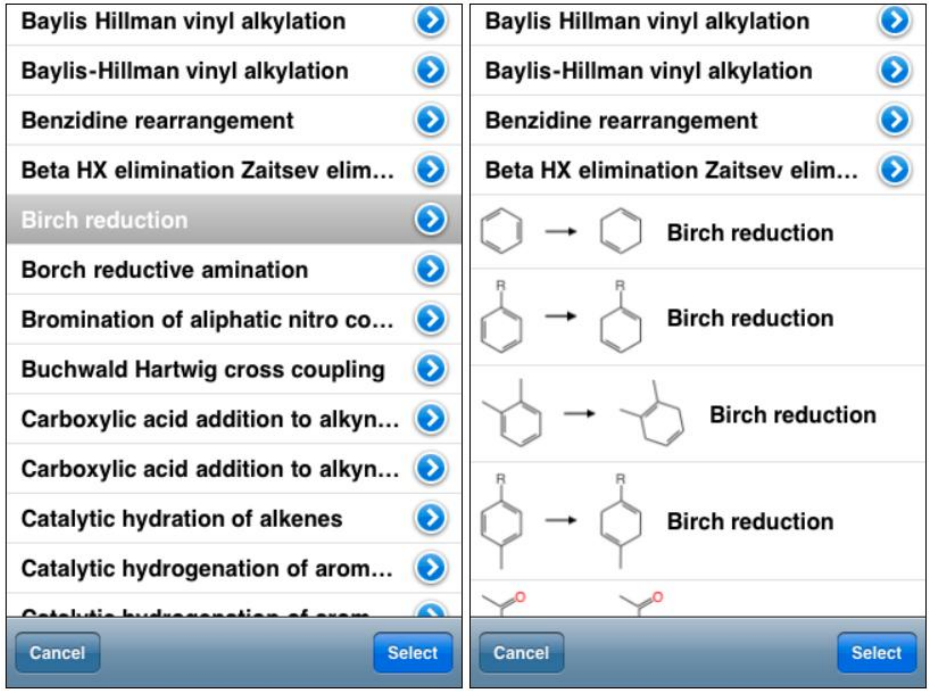
Reaction101

http://molmatinf.com/reaction101.html





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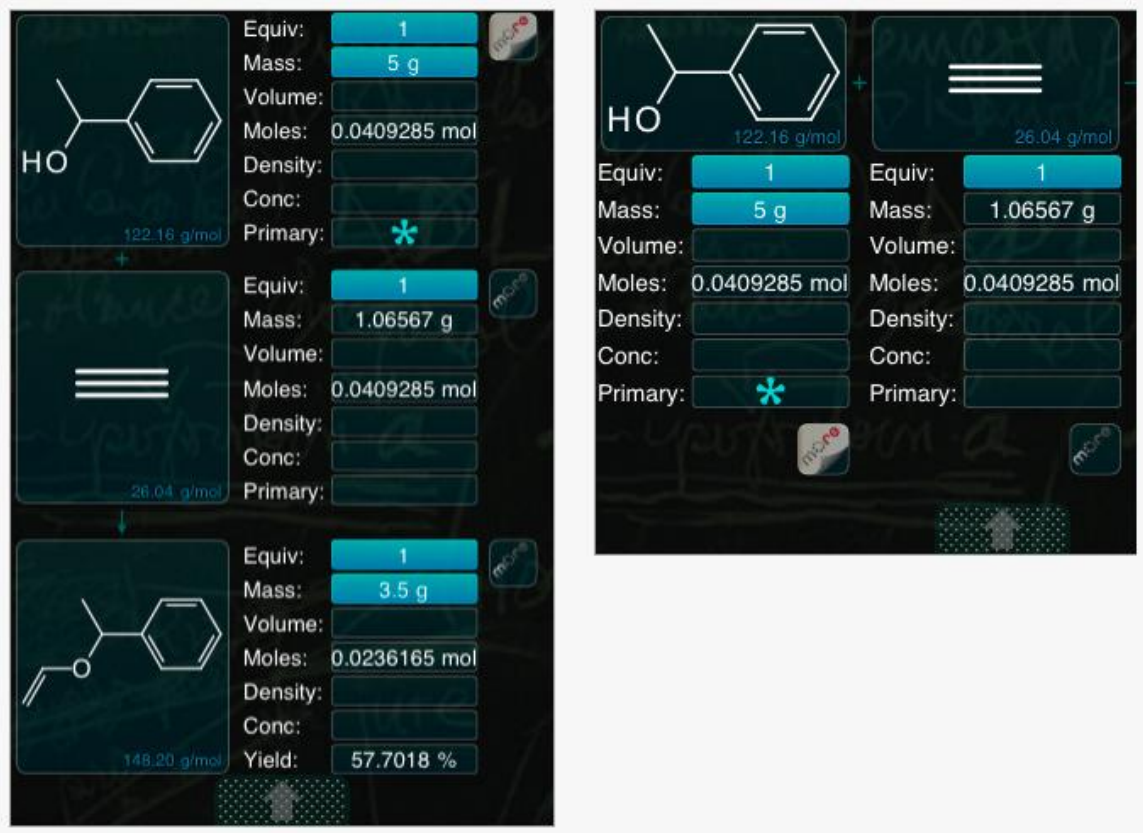
Yield 101

http://molmatinf.com/yield101.html



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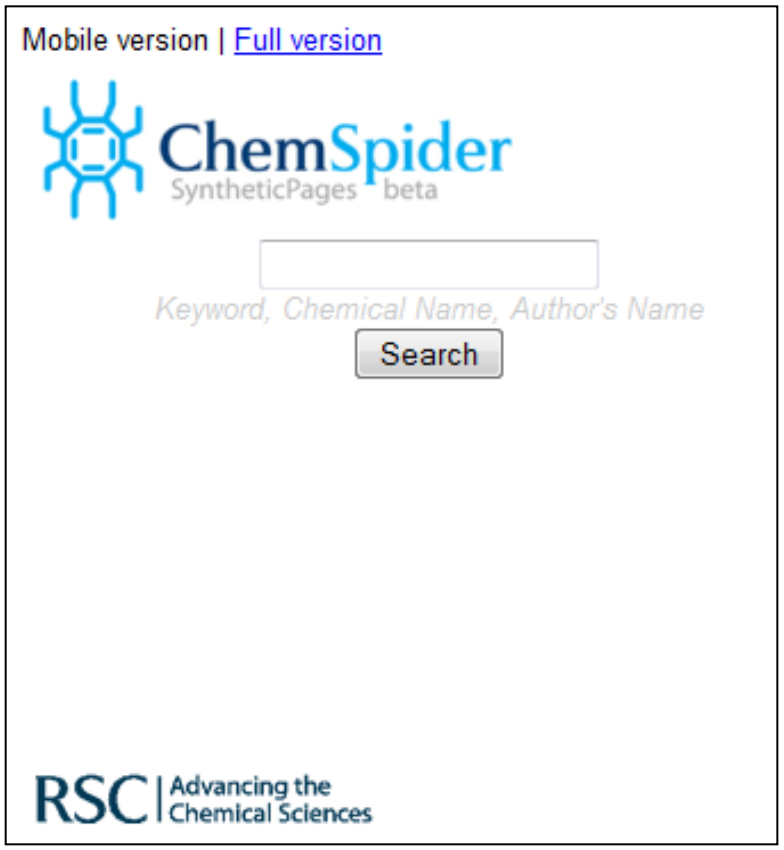
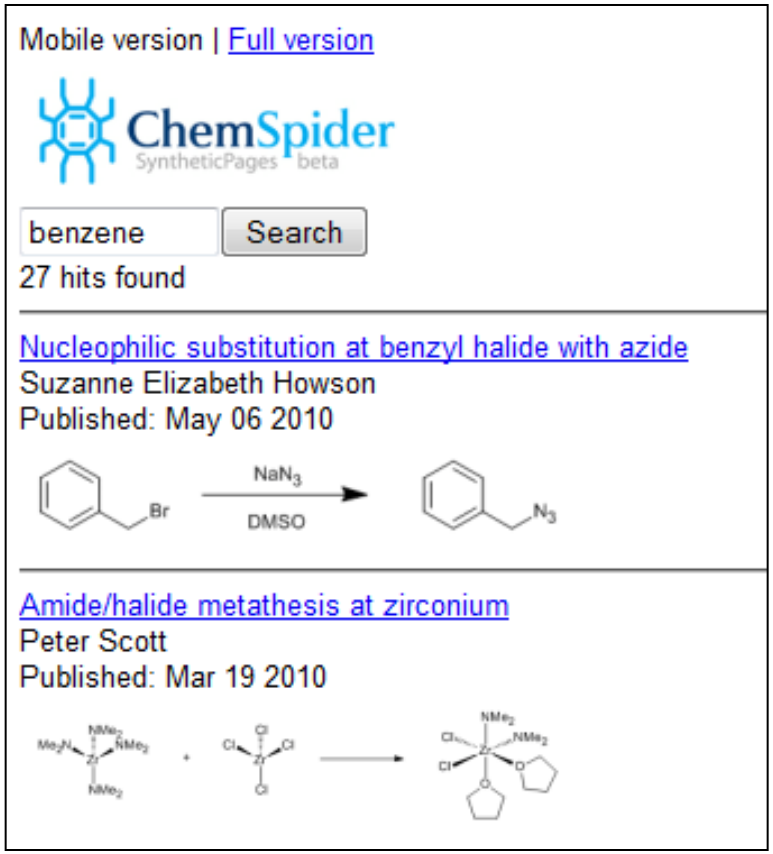
Reaction Database Look-up





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Reaction Database Look-up

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ChemSpider SyntheticPages beta

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

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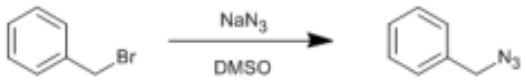
DOI: 10.1039/SP408
Submitted May 06, 2010, published May 06, 2010

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

^{1}H NMR (400 MHz, 298 K, $CDCl_3$) 7.42-7.32 (5H, m, Ph), 4.35 (2H, s, CH_2).

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“App-Based Spectroscopy”

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

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“App-Based Spectroscopy”

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

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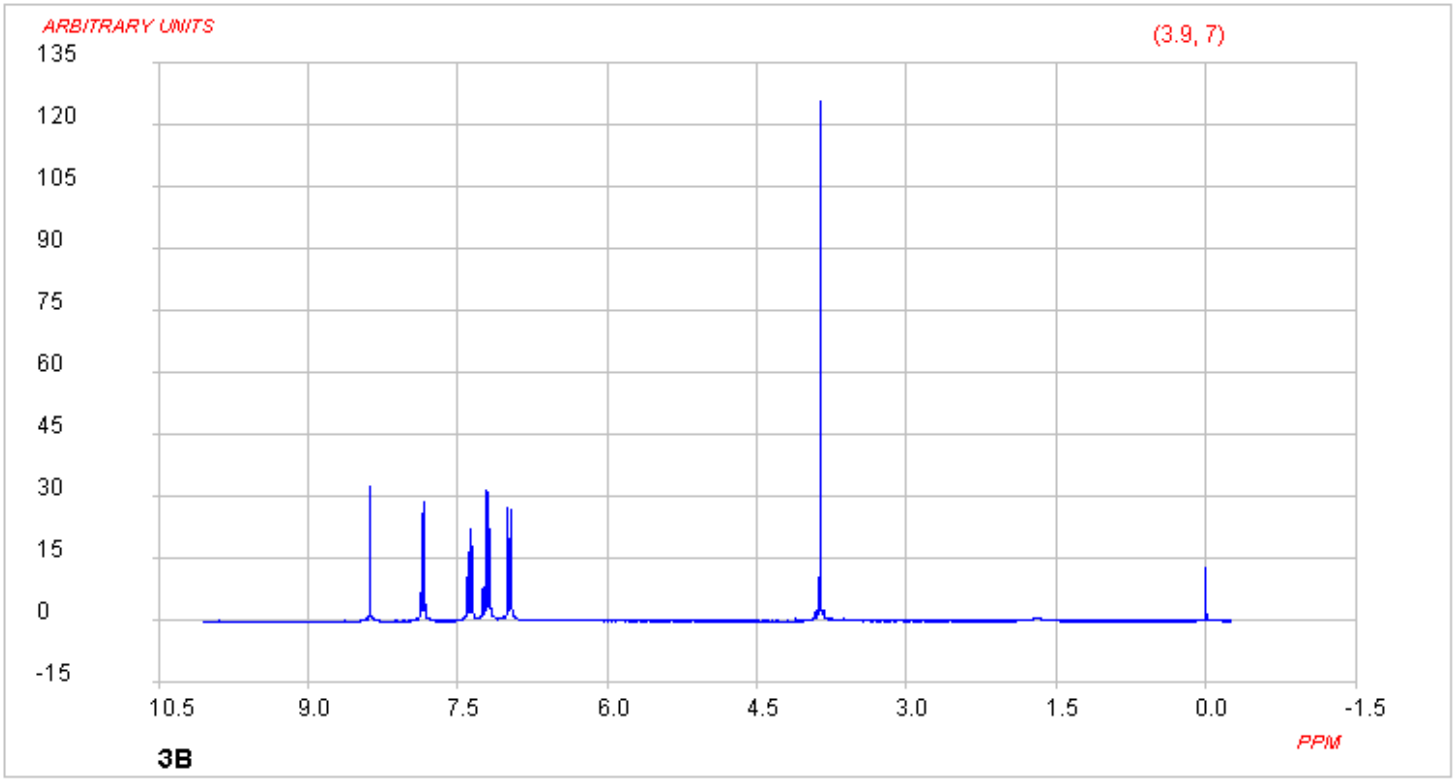
Spectra online

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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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.

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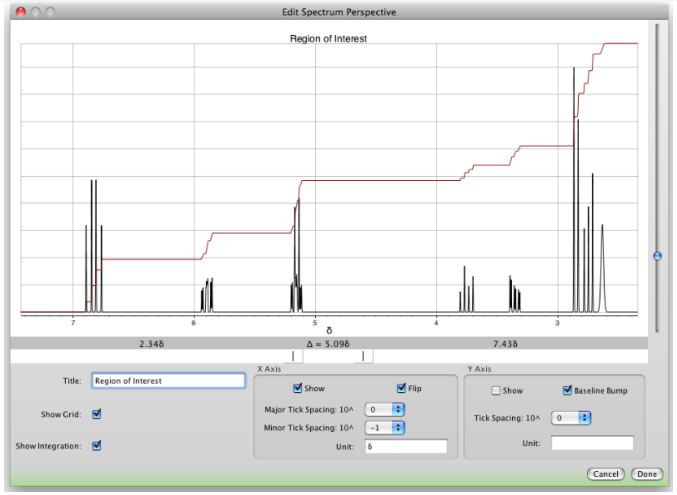
ChemDoodle
Chemical Publishing Software

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.



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Spectra in the hand

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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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Navigation

Main page
Community portal
Current events
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Random page
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Toolbox

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Upload file
Special pages
Printable version
Permanent link
Browse properties

Main Page

Contents

[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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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

ChemSpider Mobile

Company	Royal Society of Chemistry
Key people	[Dr. Antony J. Williams], Dr. Alex M. Clark
Science	Chemistry
Website	http://chemspider.com

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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.

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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

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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

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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

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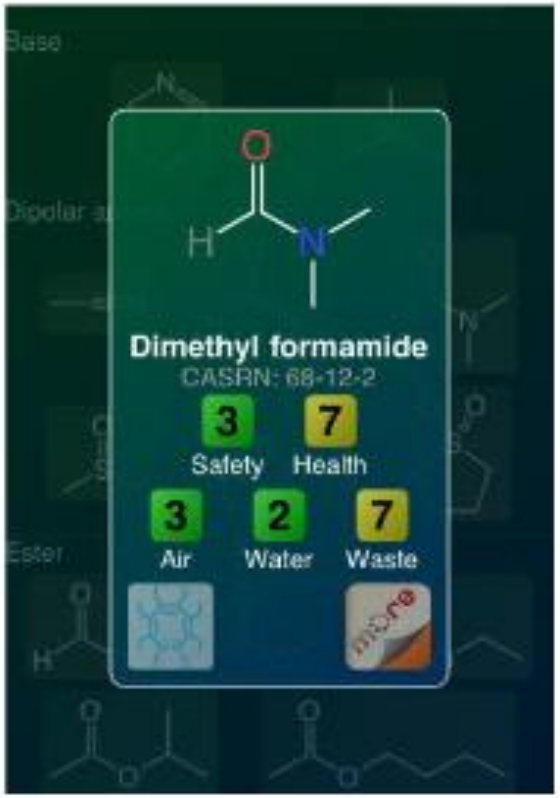
Green Solvents

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

Bad



Good

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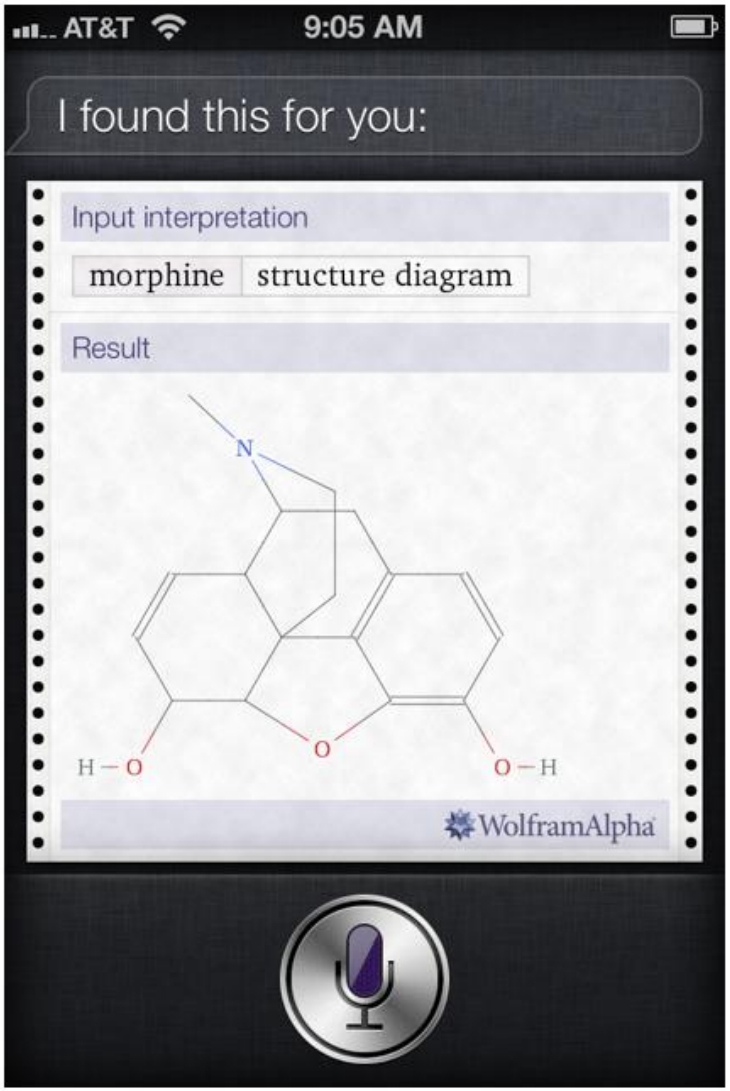
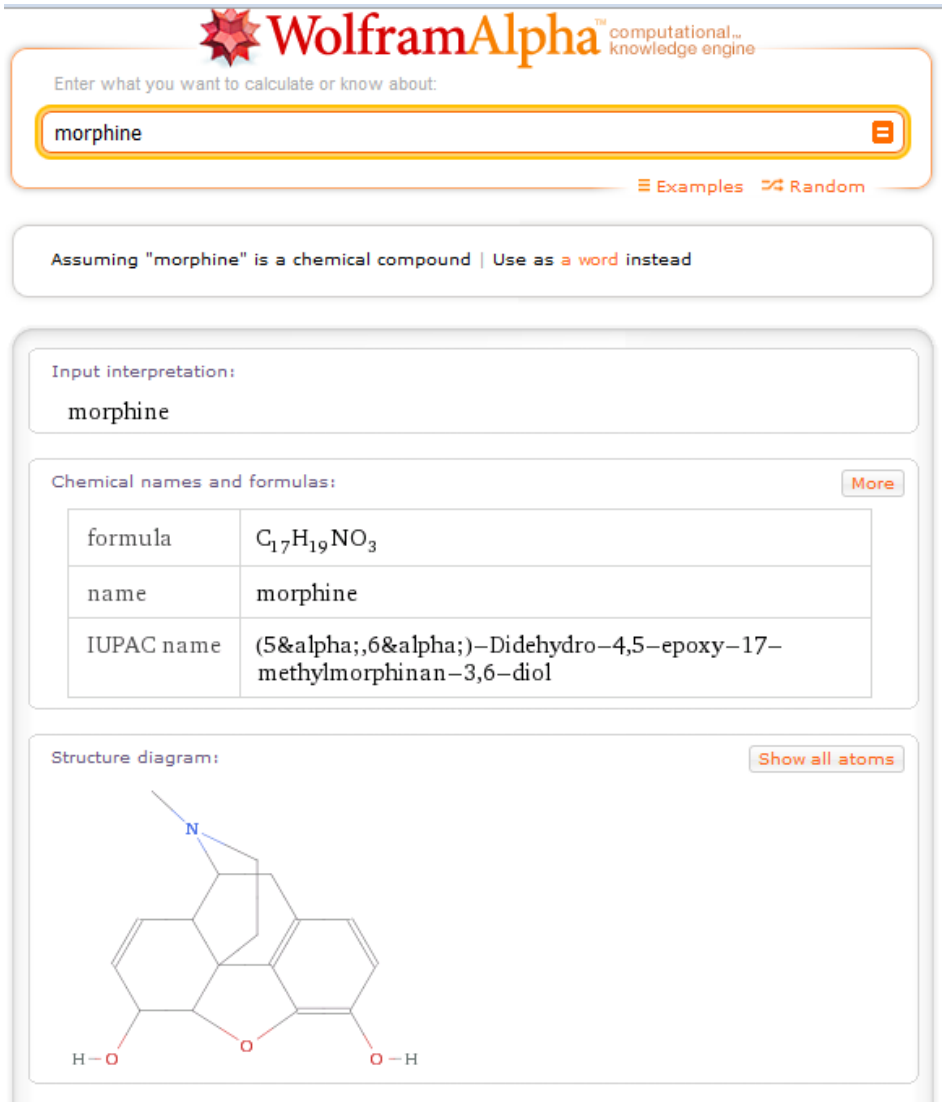
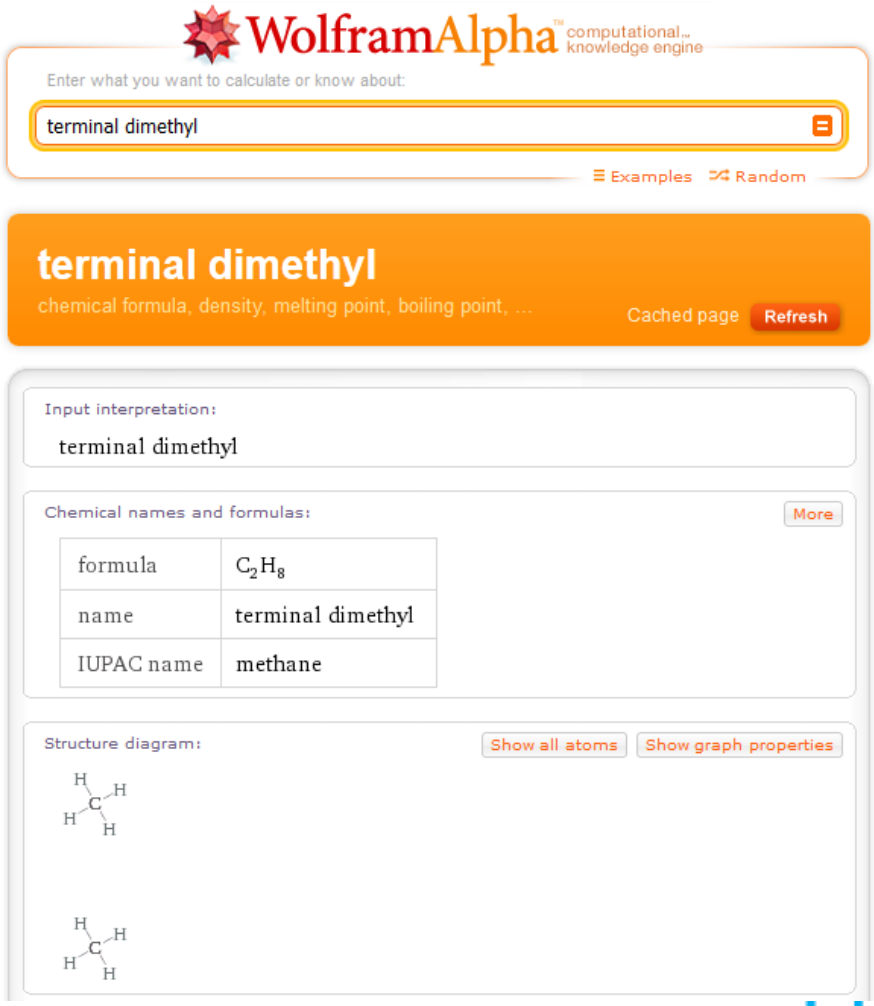
Siri ***Knows*** Chemistry???





Siri ***Accesses*** Information



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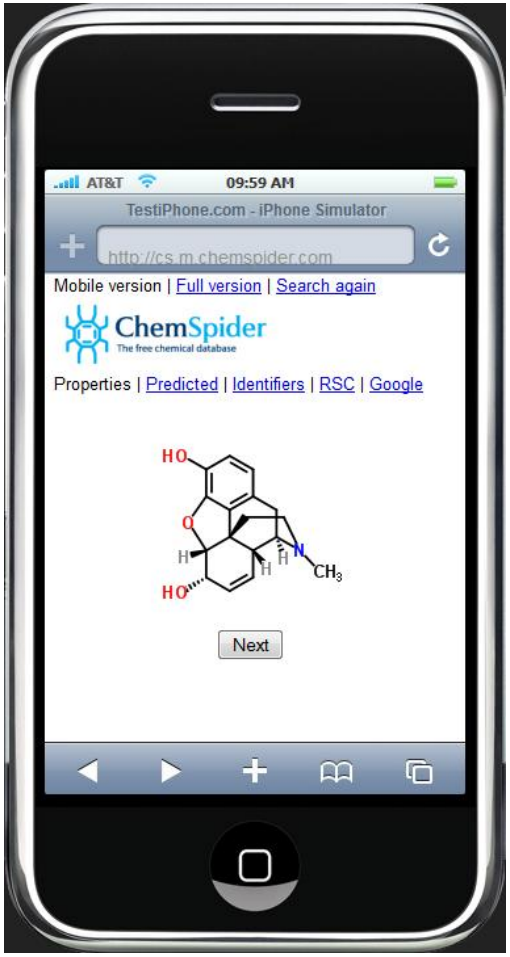
Chemists Know Chemistry



Mobile version | Full version | Search again

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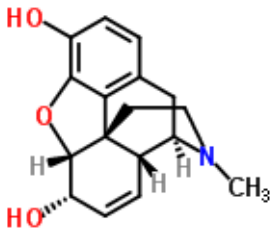
Properties | Predicted | Identifiers | RSC | Google



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Molecular Weight	285.3377
Nominal Mass	285 Da
Average Mass	285.338 Da
Monoisotopic Mass	285.137 Da
Systematic Name	
InChIKey	BQJCRHHNABKAKU-KBQPJGBKBH

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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/

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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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In Press

ELSEVIER

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. Williams[1], Sean Ekins[2], Alex M. Clark[3], J. James Jack[4] and Richard L. Apodaca[5]

[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"

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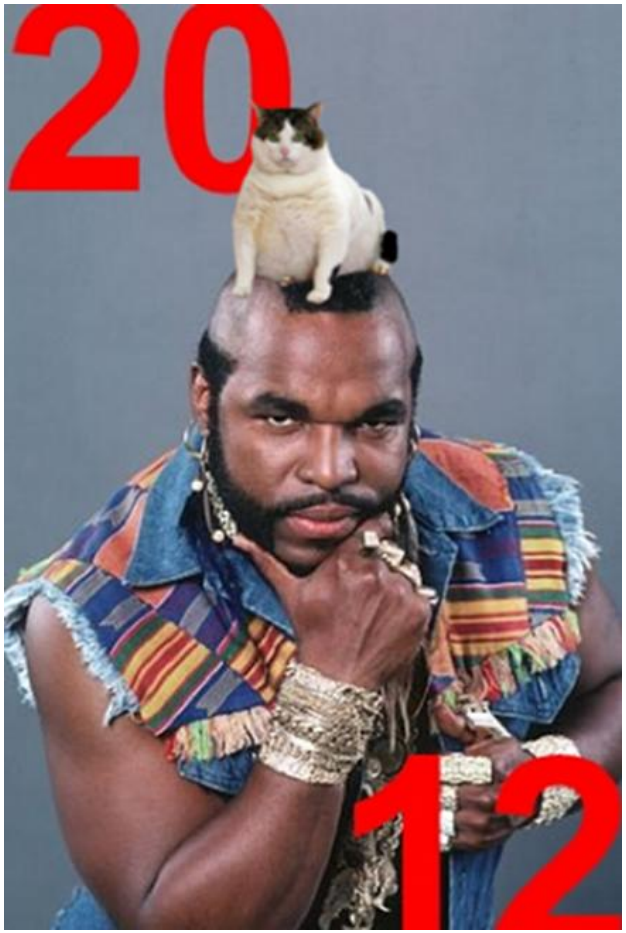
There's an "App for That"



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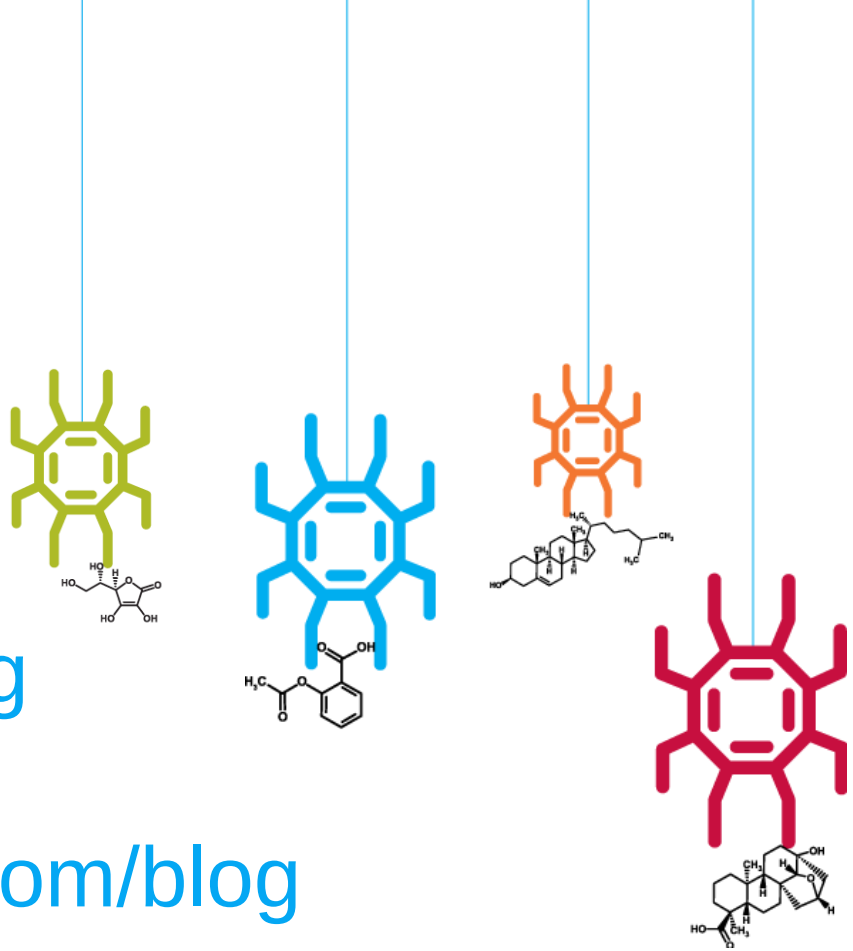
Thank you



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Personal Blog: www.chemconnector.com
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