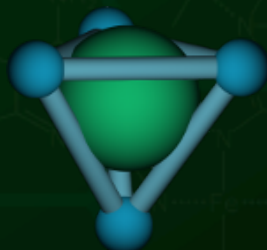


# Chemical structure diagrams, reactions and data: anytime, anywhere

**Dr. Alex M. Clark**

August 2012



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<http://molmatinf.com>

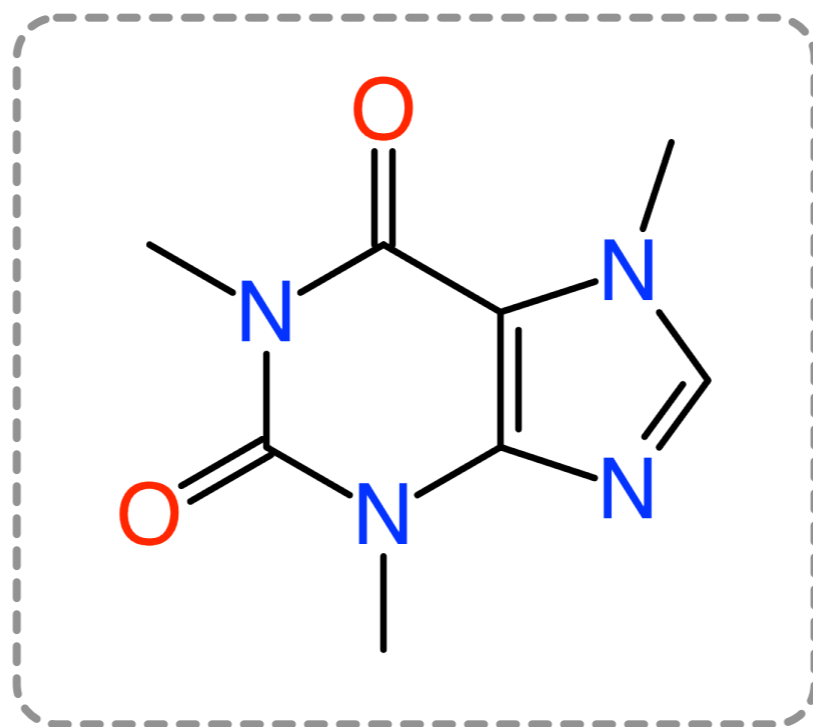
# Apps

- Already making an impact on education
- Plenty of content consumption - apps have always been good for that
- But what about content creation?
- Much harder, especially for chemical structures

# Draw a molecule

- Being able to specify a molecule opens doors

Is it valid?



Present it

Obtain  
properties

Lookup in  
catalog

Share it

# MolPrime<sup>+</sup>



- Available for iOS, with Android coming soon

# Sketching

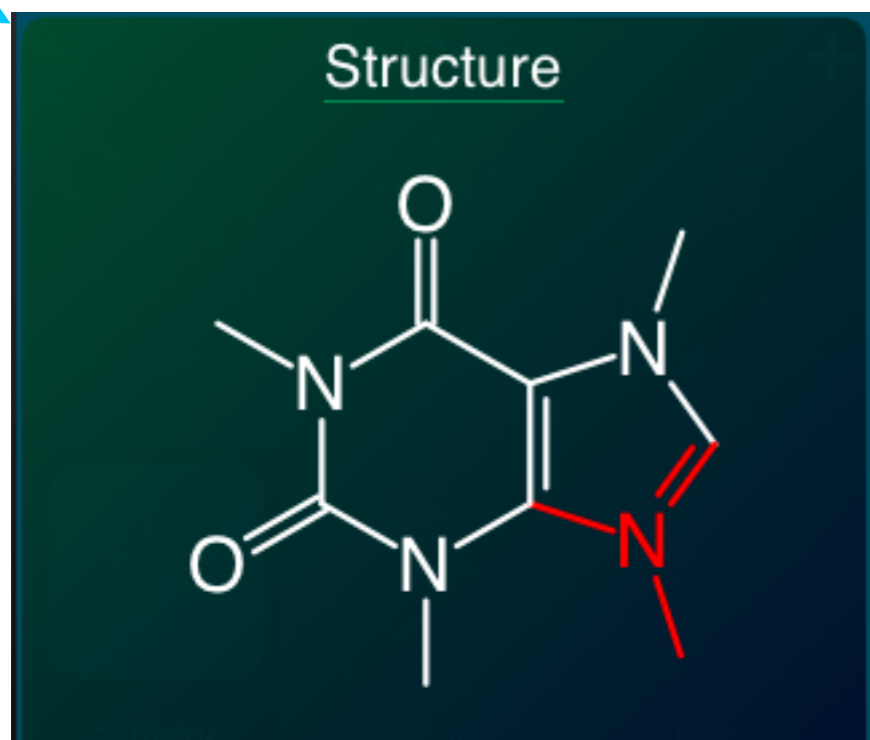


- Sketcher is designed for optimal use on small screens
- Gestures, tools, templates: for drawing *perfect* structures, with minimum interaction
- Basic primitives for molecular diagram sketching, *Journal of Cheminformatics*, **2**:8 (2010)

# Validity

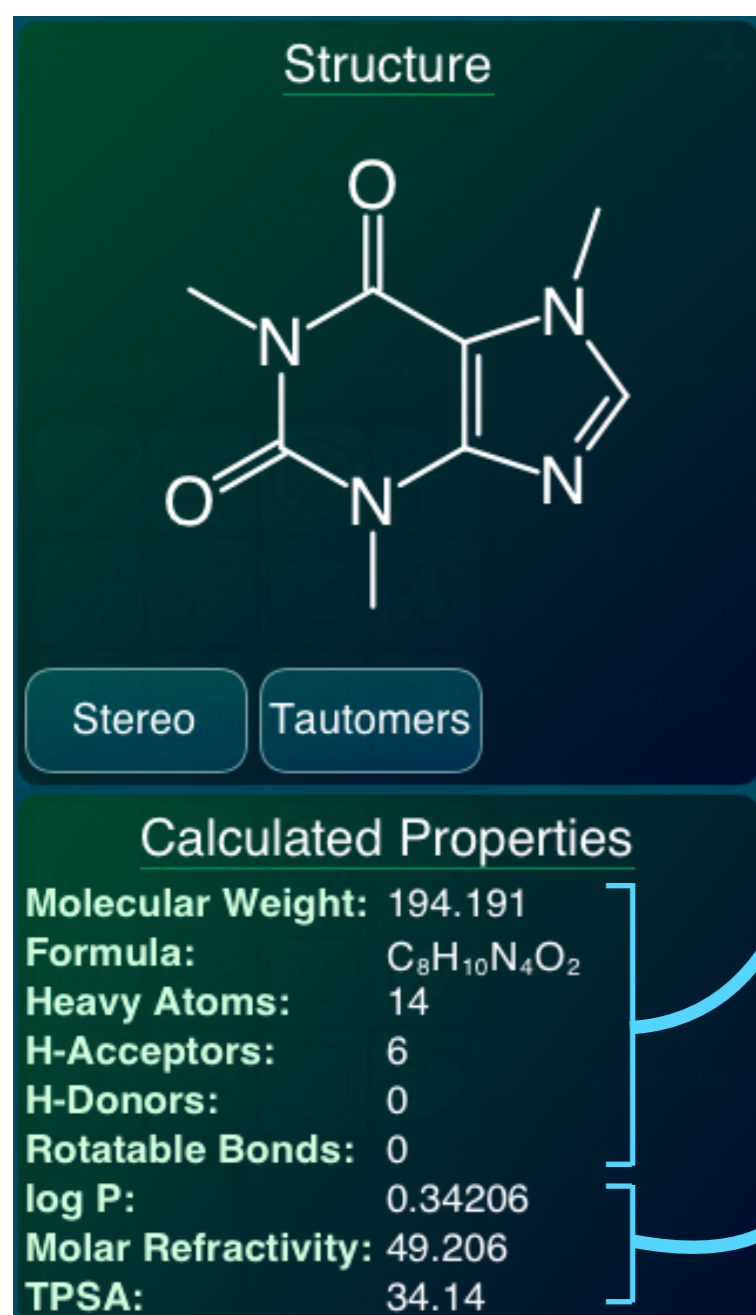


- Property calculation includes valence checking
- Identify basic problems with structures
- Drawing errors or chemistry misunderstandings lead to invalid oxidation states



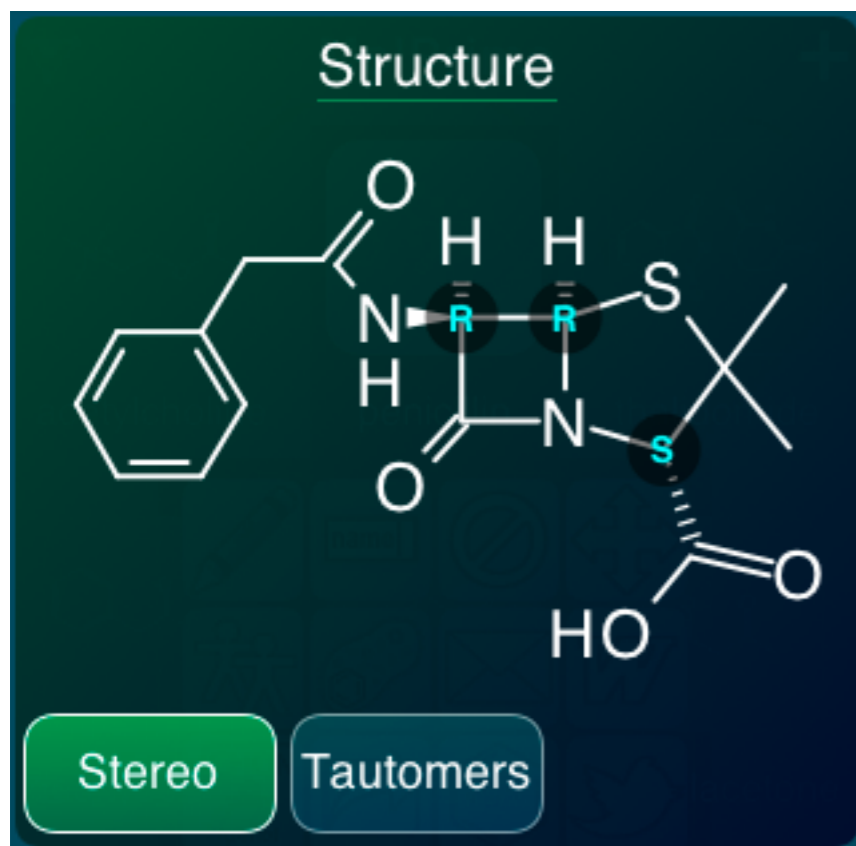
# Properties

- Scalar properties can be derived from the structure...



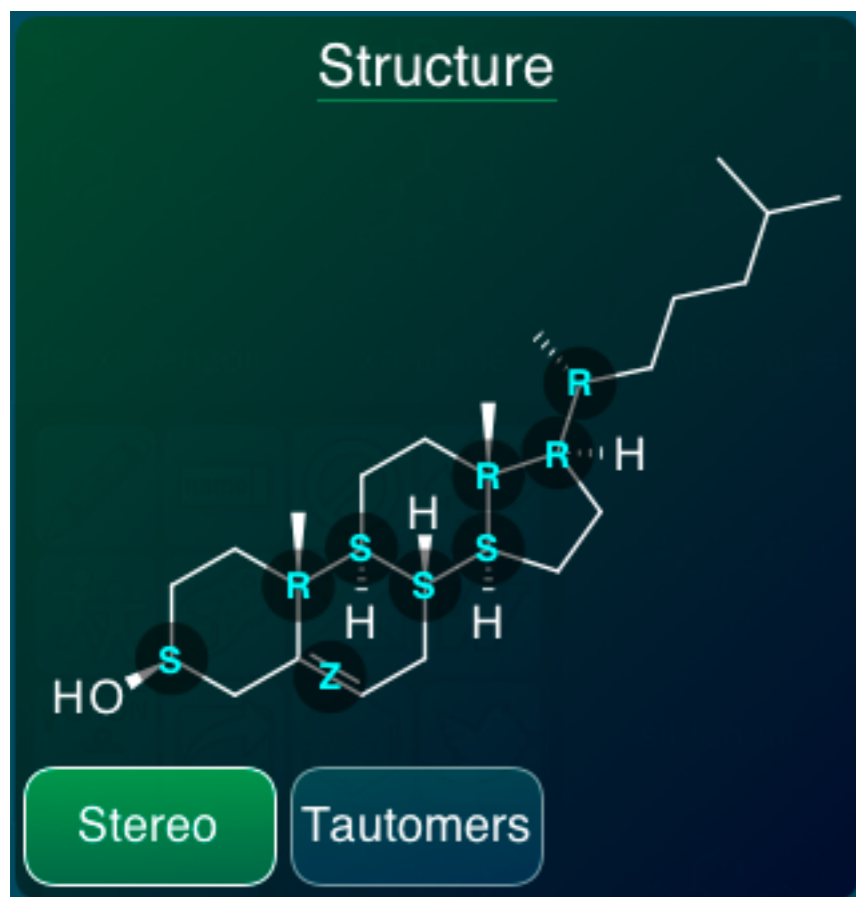
- Simple properties are calculated on the device:
  - molecular formula & weight
  - atom-type counts
  - rotatable bonds
- Detailed calculations via webservice:
  - log P
  - molar refractivity
  - topological polar surface area

# Stereochemistry



- Webservice for calculating stereochemistry:

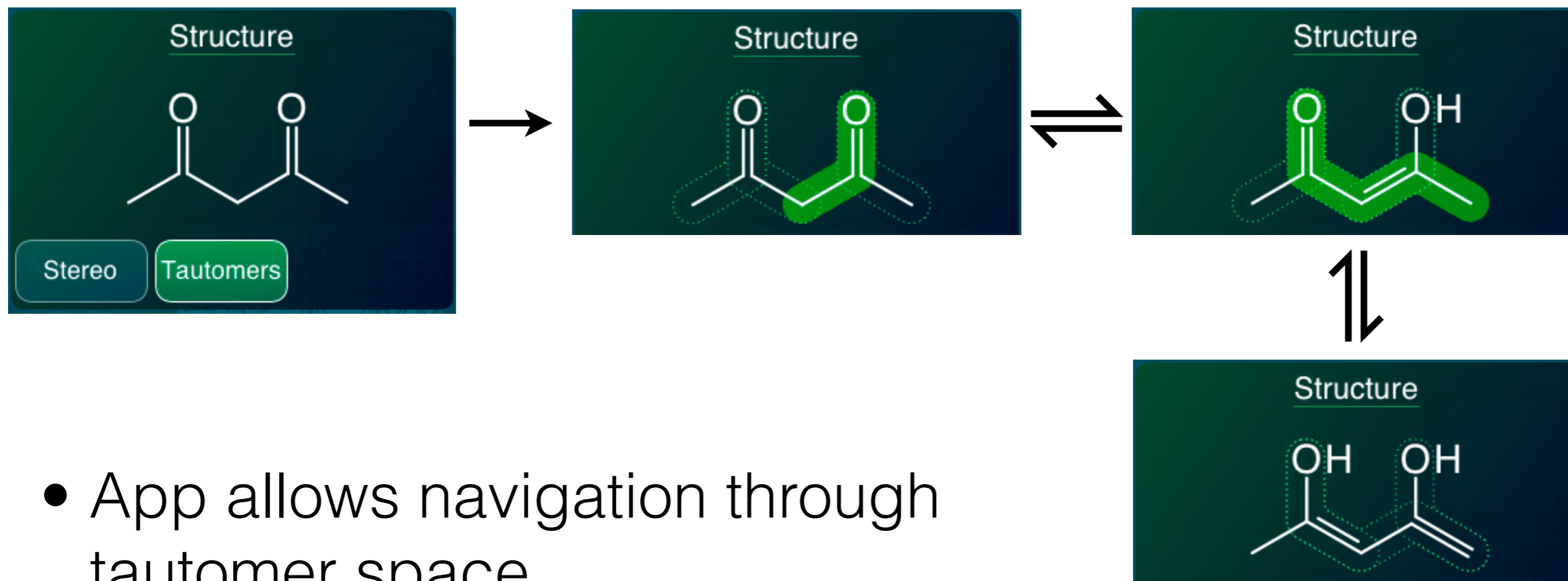
- chirality (R/S)
- double bonds (E/Z)



- Use the app to draw the molecule and obtain the correct answer

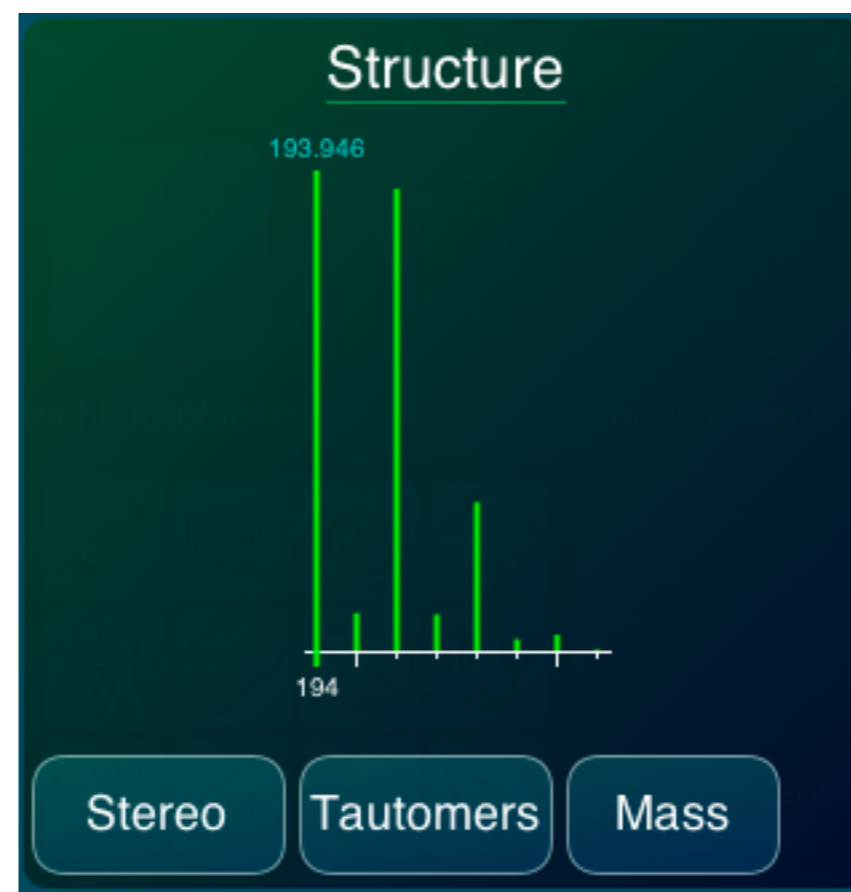
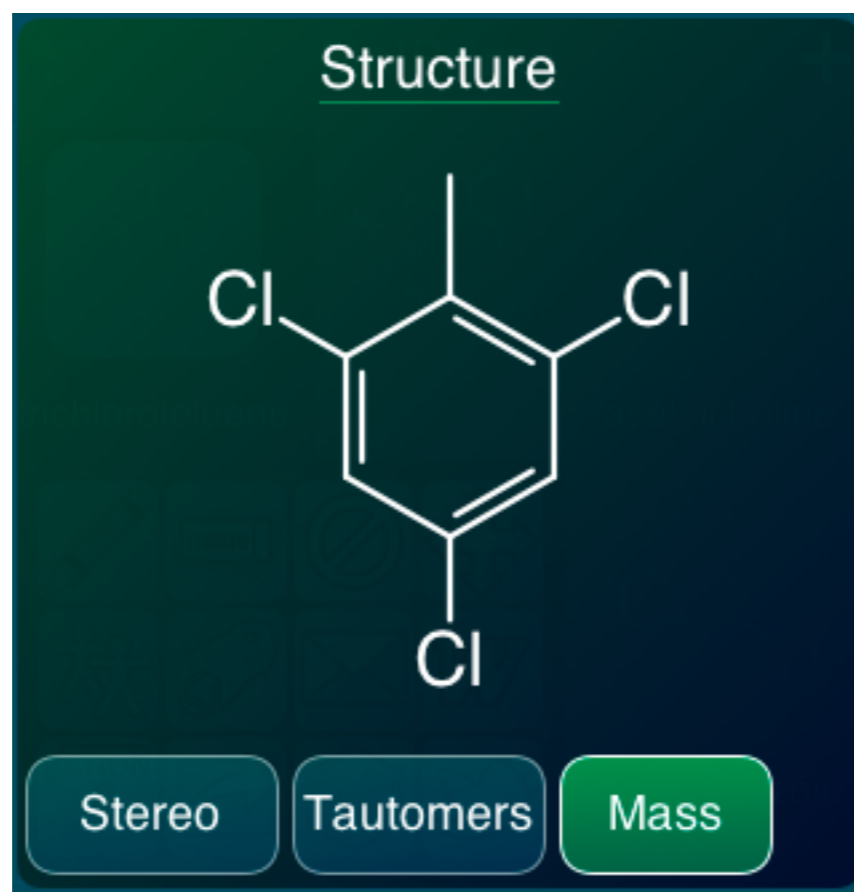
# Tautomers

- Webservice can calculate tautomers and provide an interconversion graph



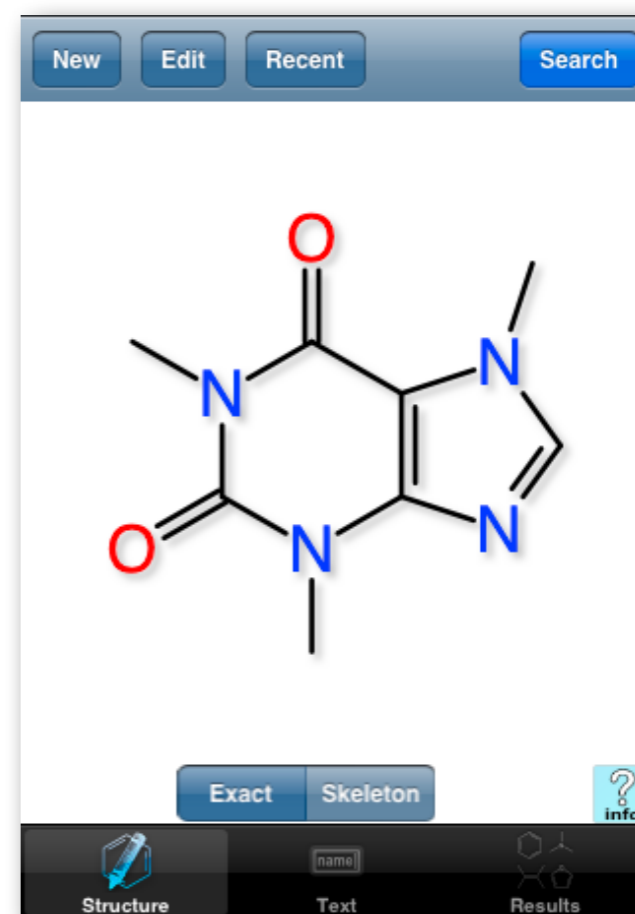
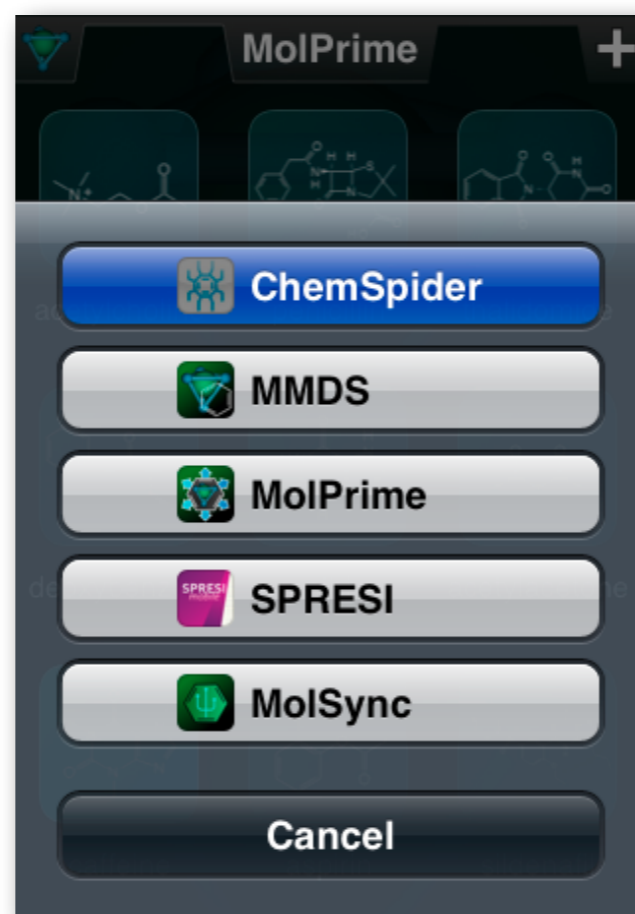
- App allows navigation through tautomer space

# Mass spectroscopy



- Can calculate the isotopic mass distribution, and exact mass, based on the structure
- Helps with assigning mass spectra

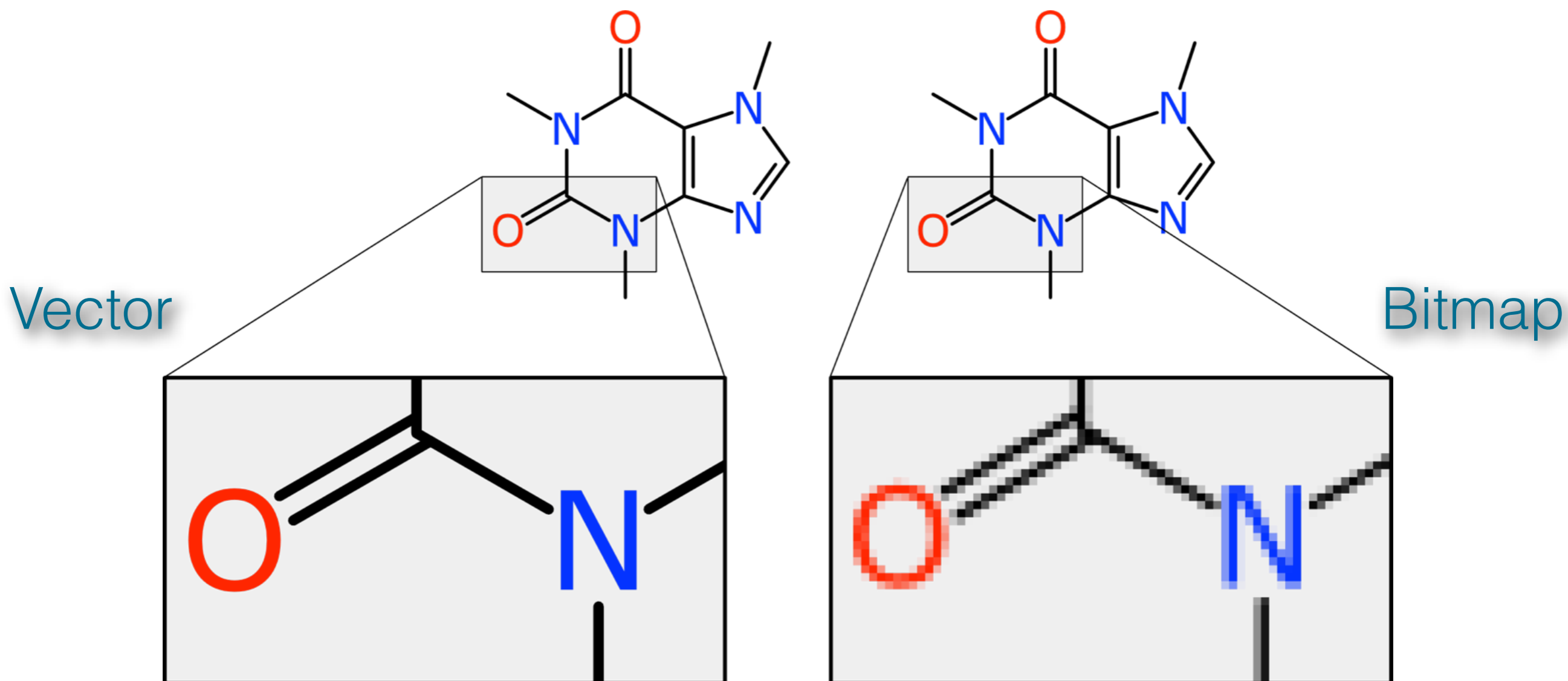
# Lookup online



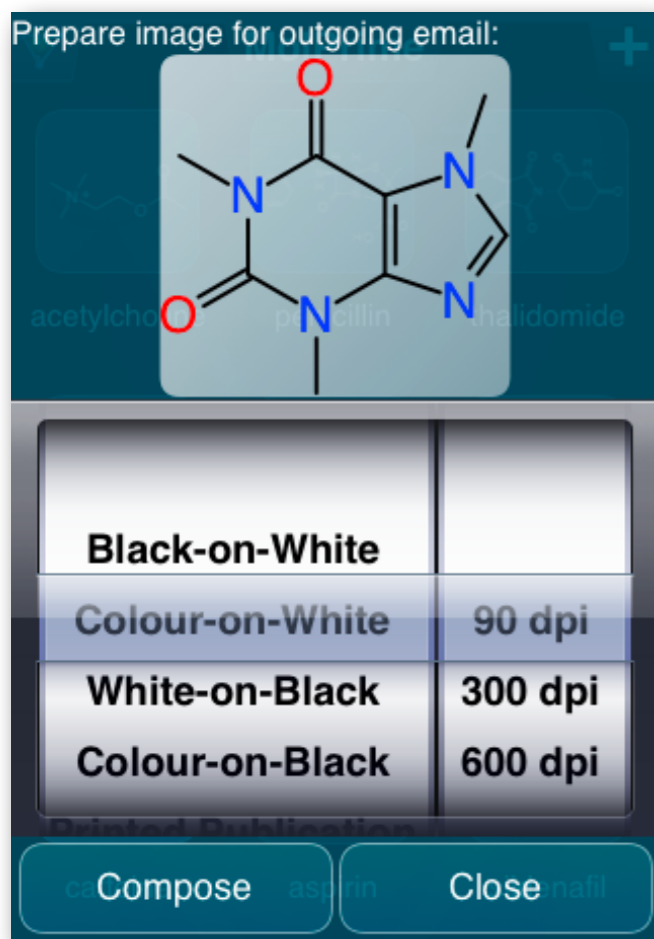
- Many ways to lookup molecular structure in online:  
e.g. Open with the ChemSpider Mobile app
- Can also search SPRESI, Mobile Reagents, PubChem, ChEBI, eMolecules

# Presentation

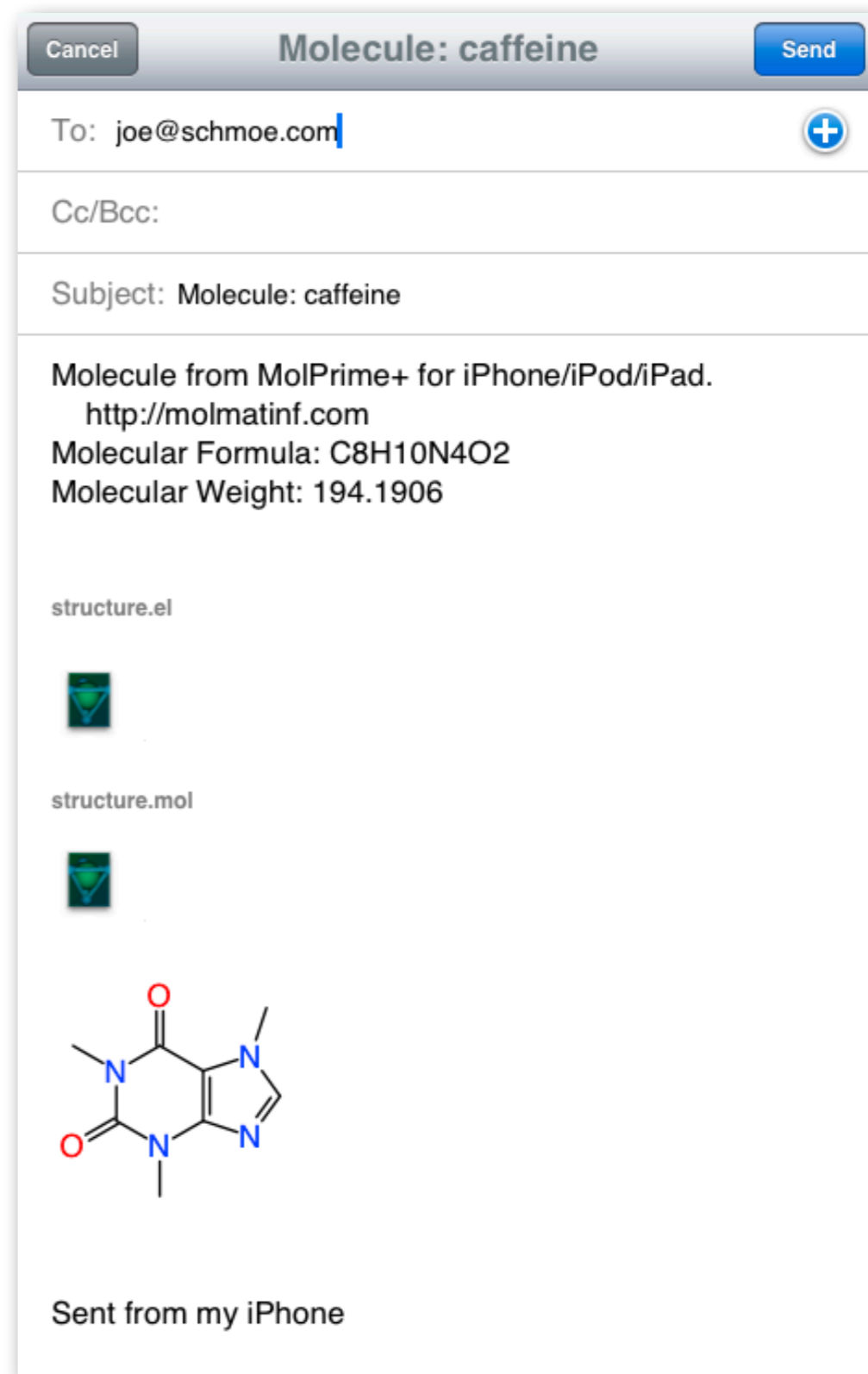
- Can copy bitmap to clipboard: paste into iWork
- Or create **vector graphics** (SVG, EPS, Word/Excel)



# Sharing: Email



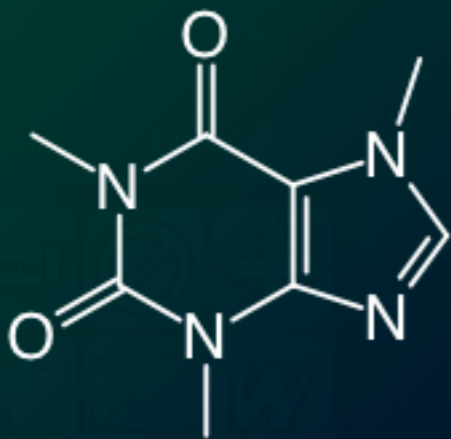
- Initiate an email, with an image, source data...



- Recipient can view the picture...
- ... and open the data: with an app, or any other platform software.

## Upload

Prior to sharing on the web, your content needs to be uploaded to <http://molsync.com/MolSync>



Upload

## Link

Public link:  
<http://molsync.com/share?mol=1993>

caffeine

aspirin

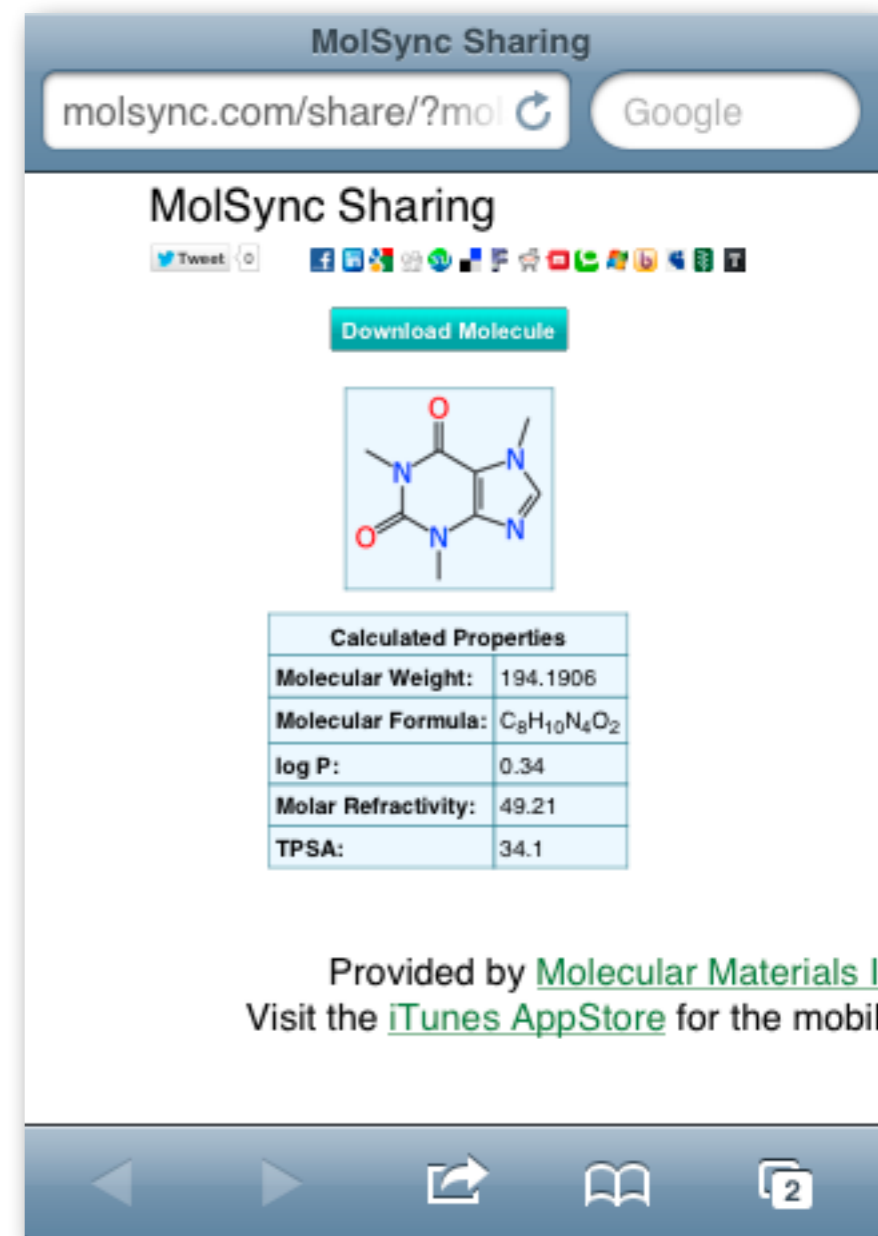
Close

# Sharing: Web

- Upload to **molsync.com**

- View public link

- Can share the link with anyone, e.g. via social networks
- Can download the structure in many formats, including graphics

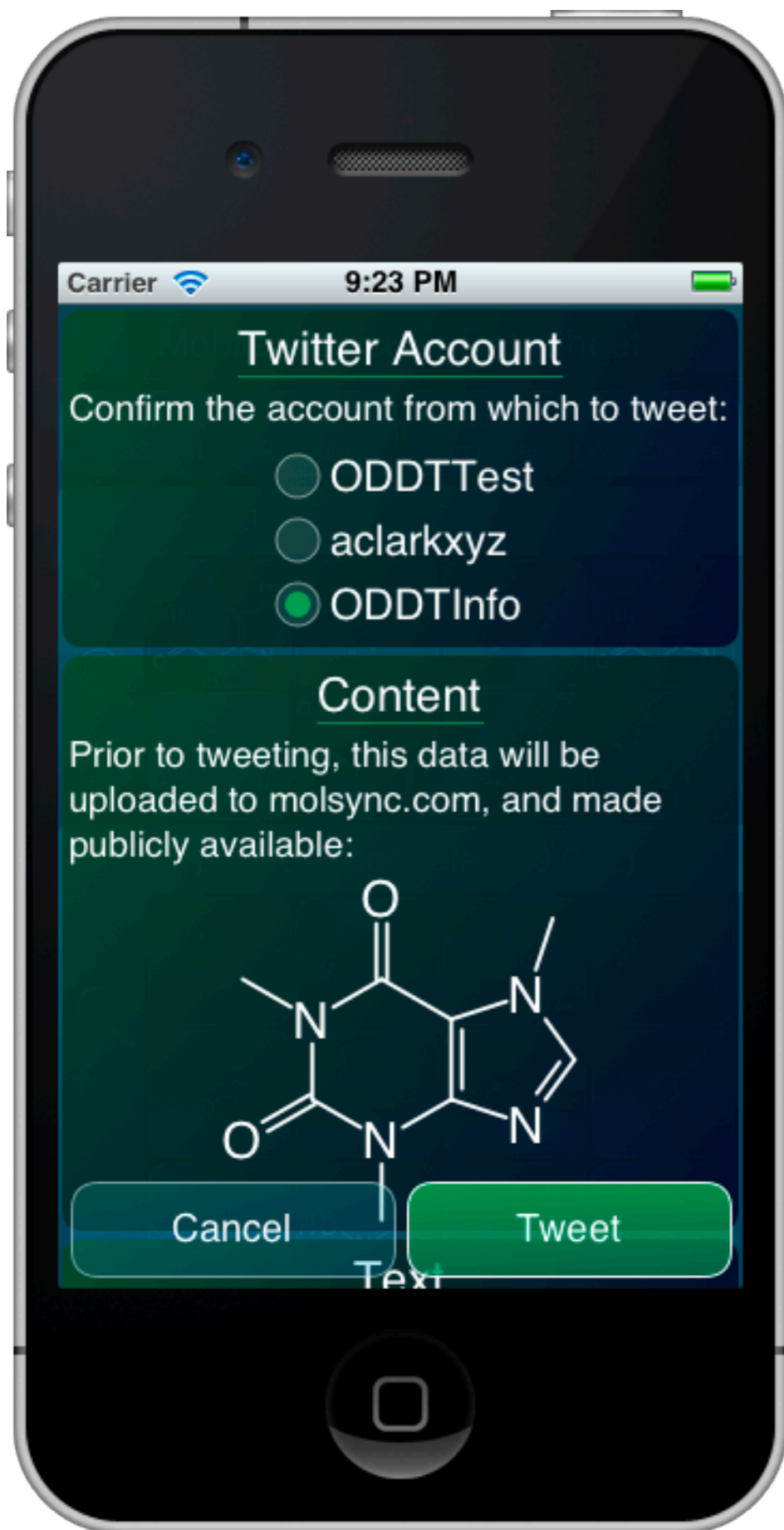


The screenshot shows the MolSync Sharing web interface. At the top, there is a search bar with the URL [molsync.com/share/?mol](http://molsync.com/share/?mol) and a Google search button. Below the search bar, the page title is "MolSync Sharing". There are social media sharing icons for Twitter, Facebook, LinkedIn, and others. A "Download Molecule" button is visible. The main content area displays the chemical structure of caffeine. Below the structure is a table of "Calculated Properties":

Calculated Properties	
Molecular Weight:	194.1906
Molecular Formula:	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>
log P:	0.34
Molar Refractivity:	49.21
TPSA:	34.1

At the bottom, there is a footer that reads "Provided by Molecular Materials | Visit the iTunes AppStore for the mobile app". The bottom navigation bar includes icons for back, forward, share, and tabs.

# Twitter



- Can tweet from app using iOS Twitter integration
- Uploads molecule to website
- Includes the link within the tweet
- Link provides viewing *and* access to the data

# See Also

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



Mobile Molecular  
DataSheet (MMDS)



MolSync



SAR Table



MolPrime



Green Solvents

Open Drug Discovery  
Teams (ODDT)

*with Collaborations in Chemistry*



ChemSpider Mobile

*with Royal Society of Chemistry*



SPRESI *mobile*

*with InfoChem*



Reaction 101

*with Eidogen-Sertanty*



Yield 101

*with Eidogen-Sertanty*



# Conclusion

- Numerous ways to teach chemistry, using molecular structures
- Useful pedagogical tools already available, starting with structure drawing
- This is just the beginning... so many more ideas to explore.

<http://molmatinf.com>

<http://molsync.com>

<http://cheminf20.org>

@aclarkxyz

