Chemical structure diagrams, reactions and data: anytime, anywhere

Dr. Alex M. Clark

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http://molmatinf.com

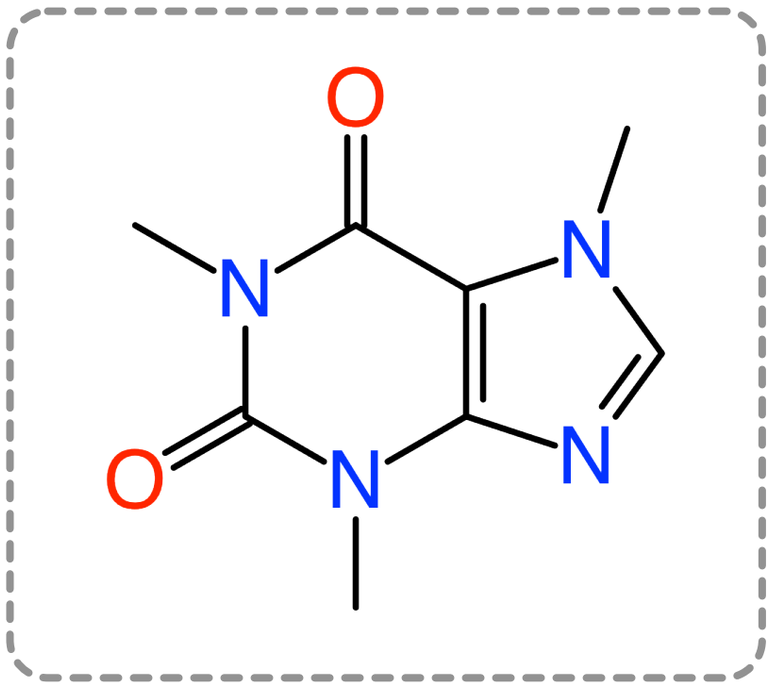
Apps

- 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?



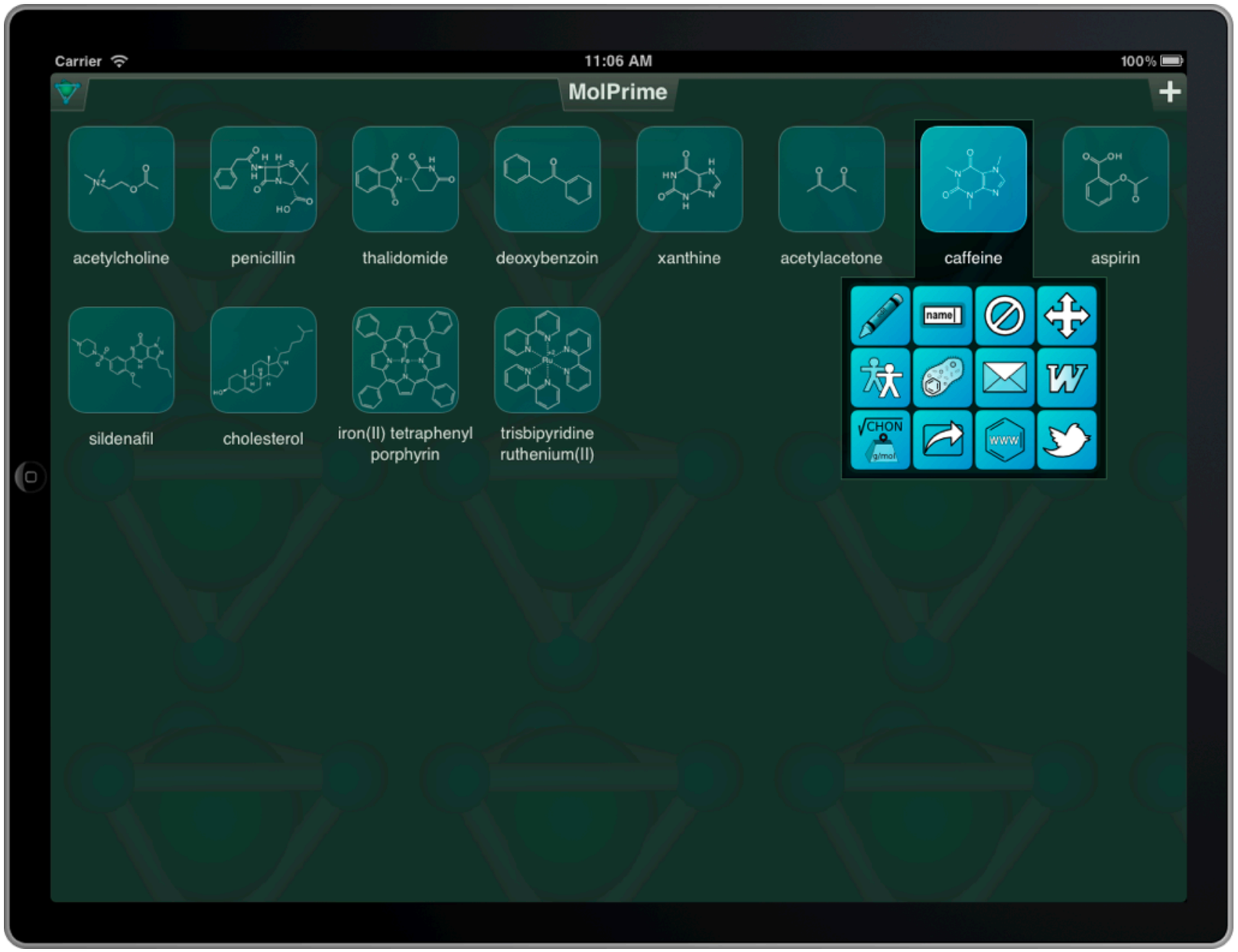
Present it

Obtain properties

Lookup in catalog

Share it

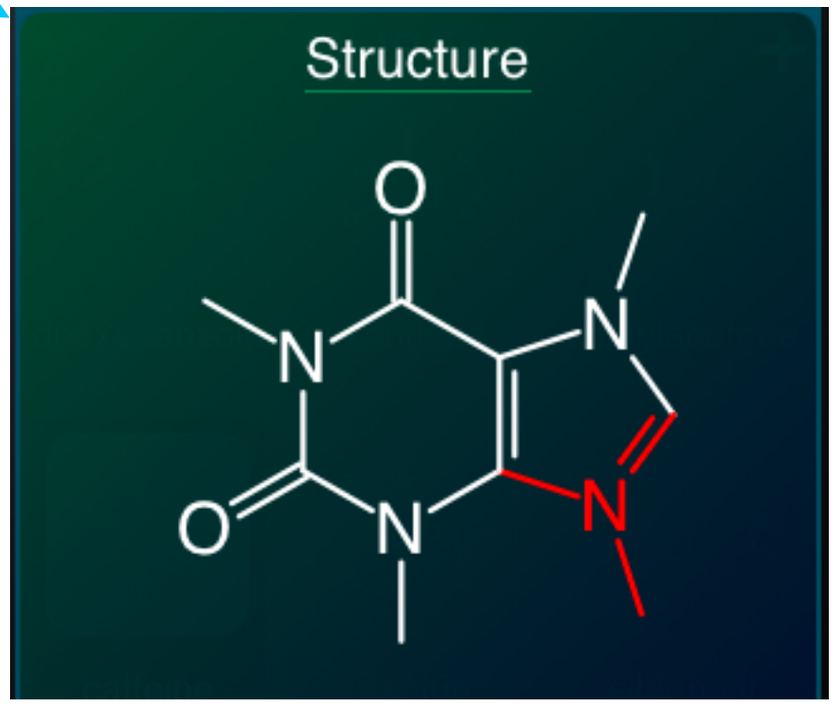
MolPrime+



- 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)

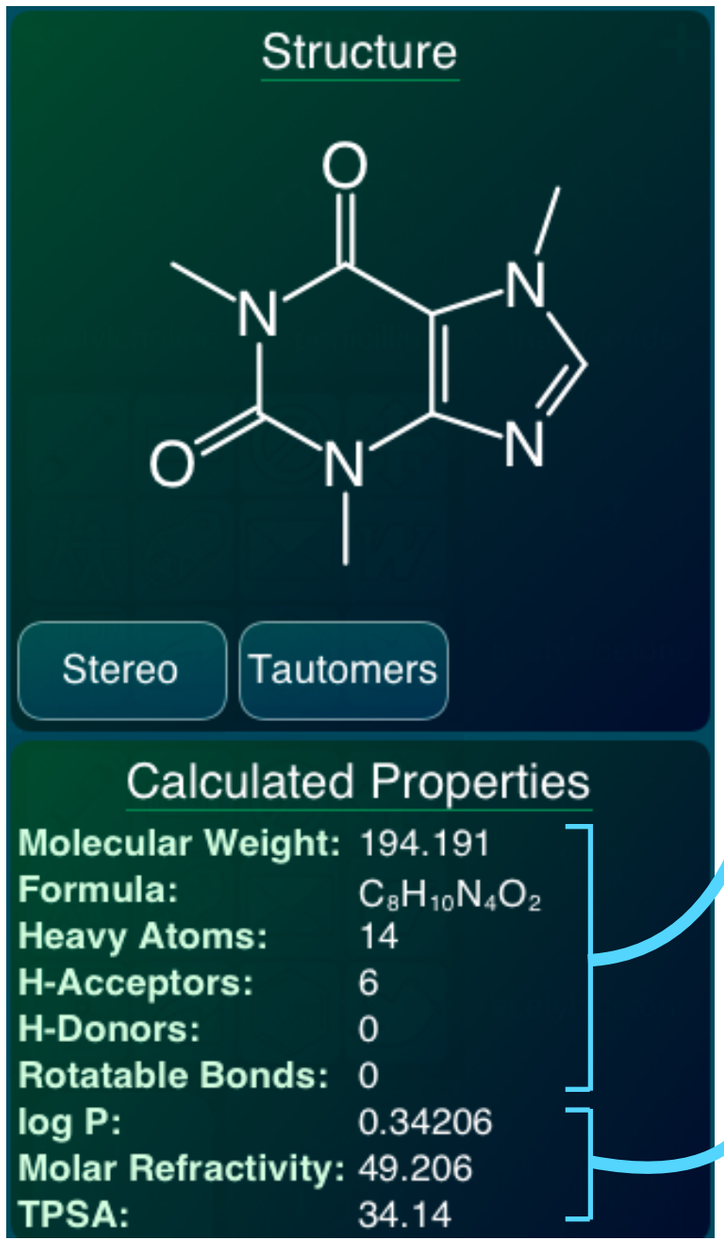


Validity

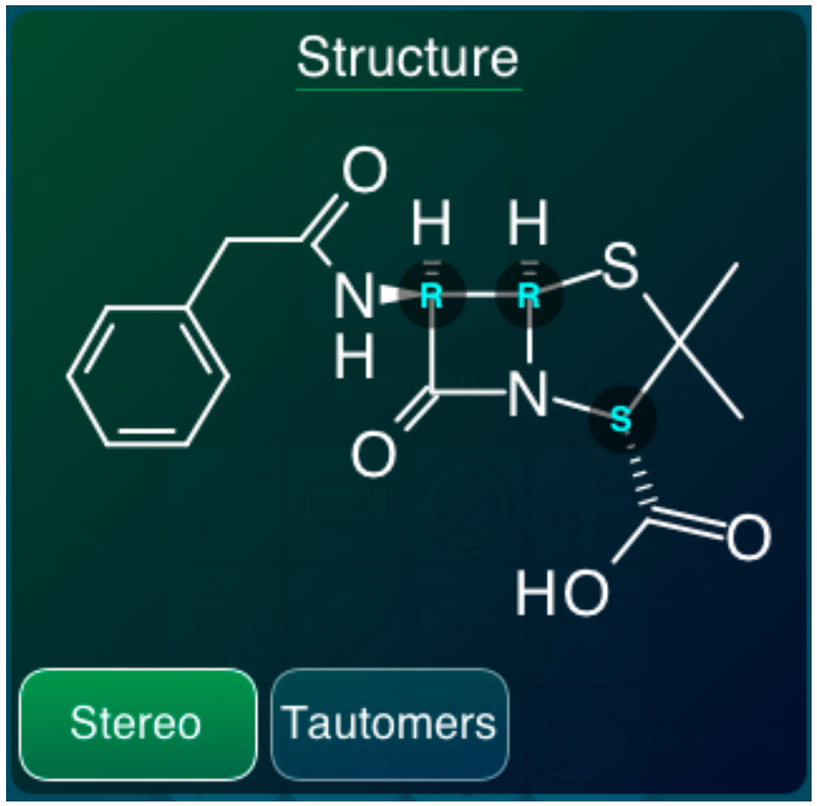
- Property calculation includes valence checking
- Identify basic problems with structures
- Drawing errors or chemistry misunderstandings lead to invalid oxidation states

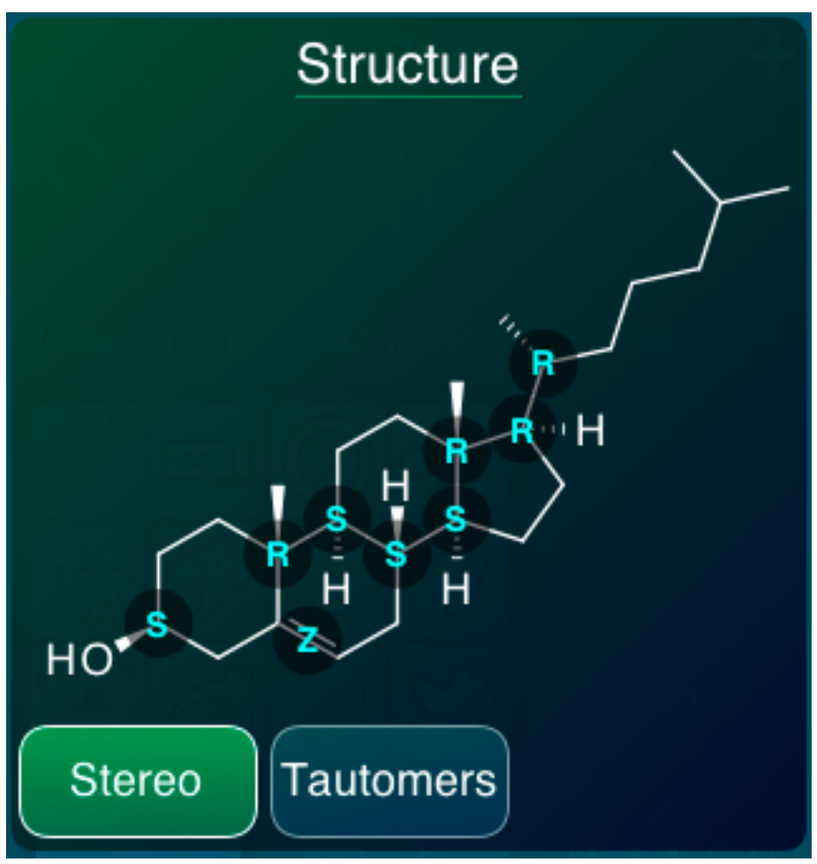
Properties

- 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





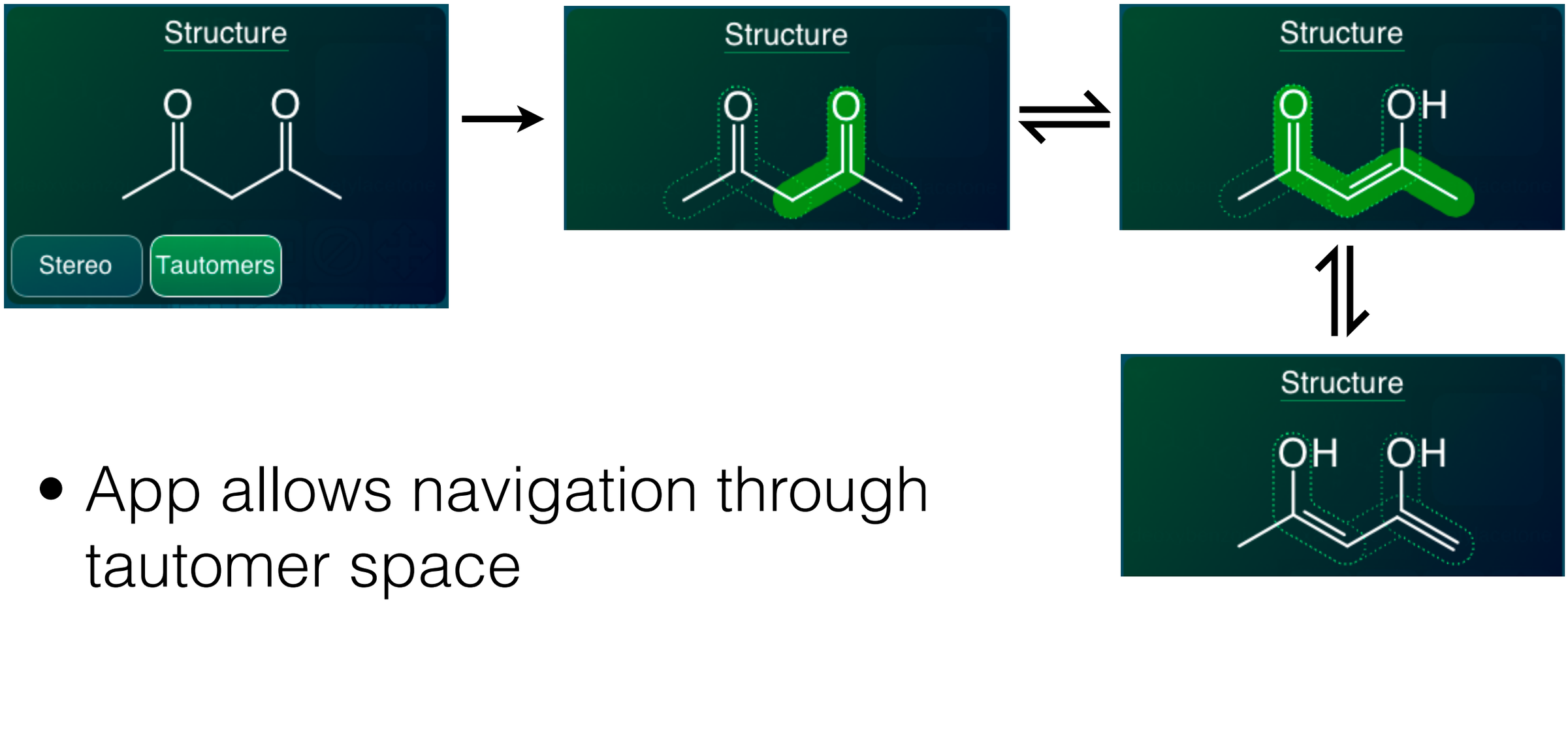
Stereochemistry

- Webservice for calculating stereochemistry:
  - chirality (R/S)
  - double bonds (E/Z)

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

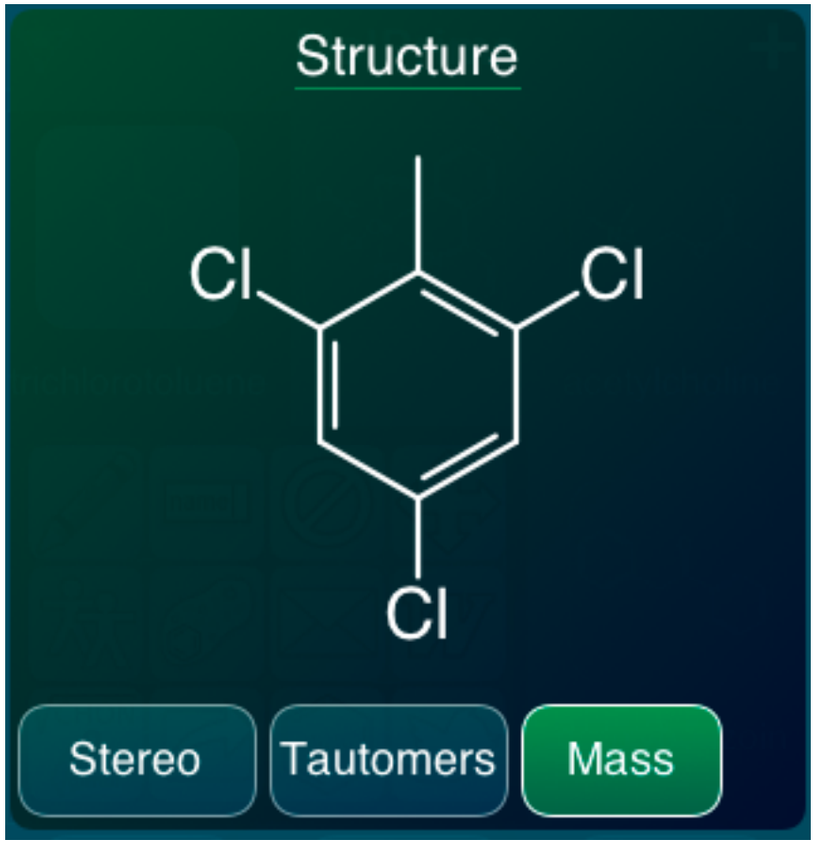
Tautomers

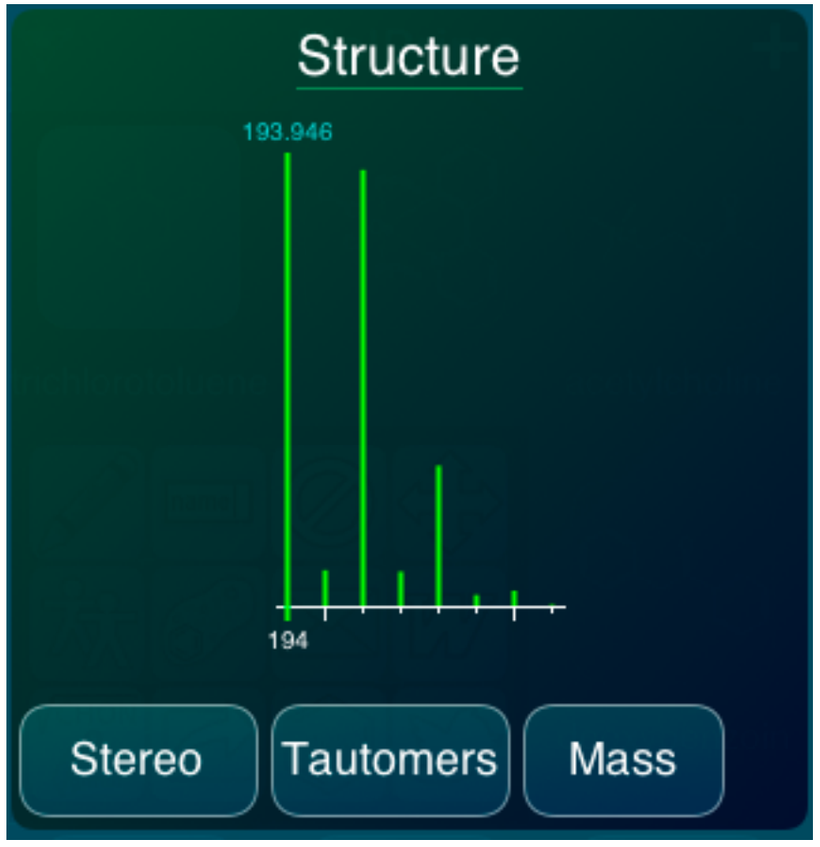
- Webservice can calculate tautomers and provide an interconversion graph



- App allows navigation through tautomer space

Mass spectroscopy

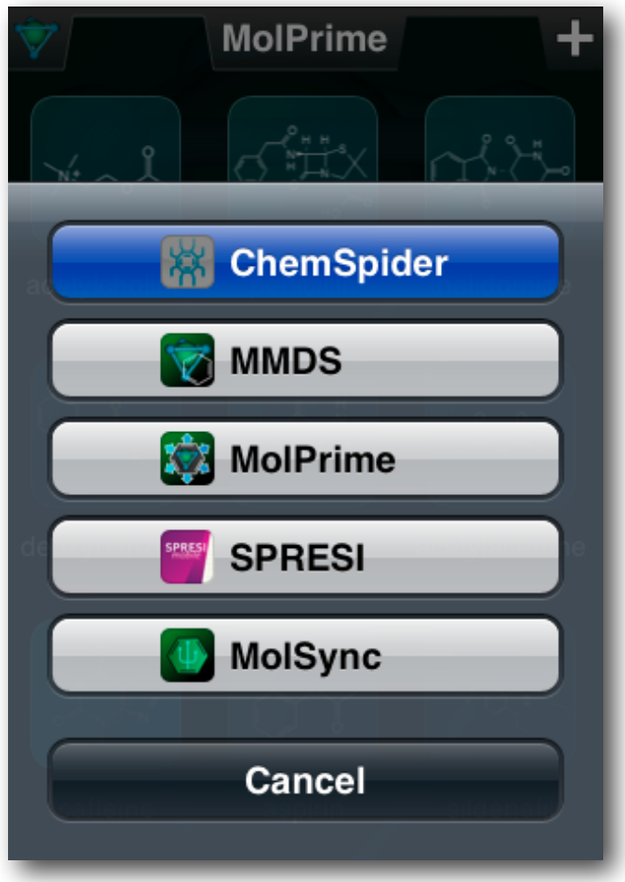


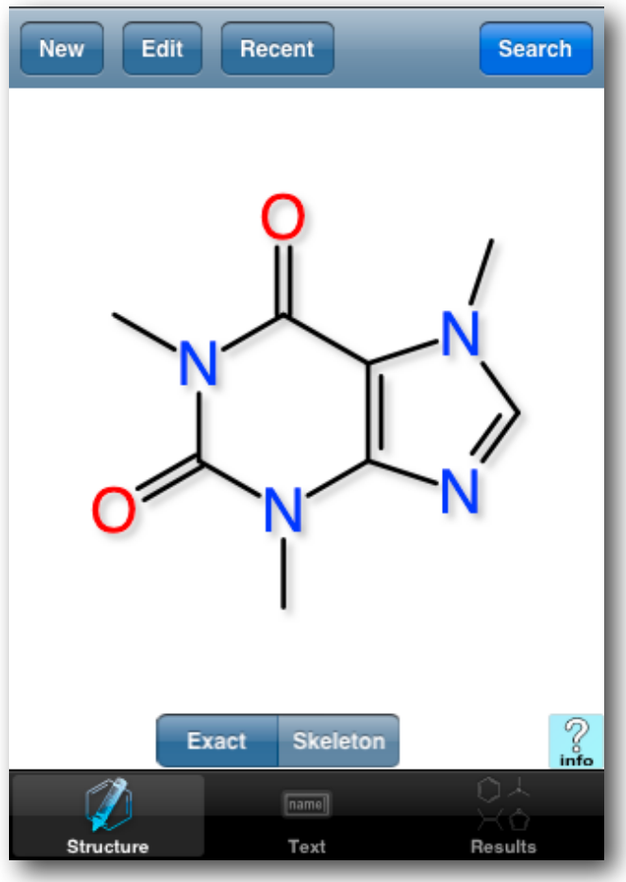


- Can calculate the isotopic mass distribution, and exact mass, based on the structure

- Helps with assigning mass spectra

Lookup online



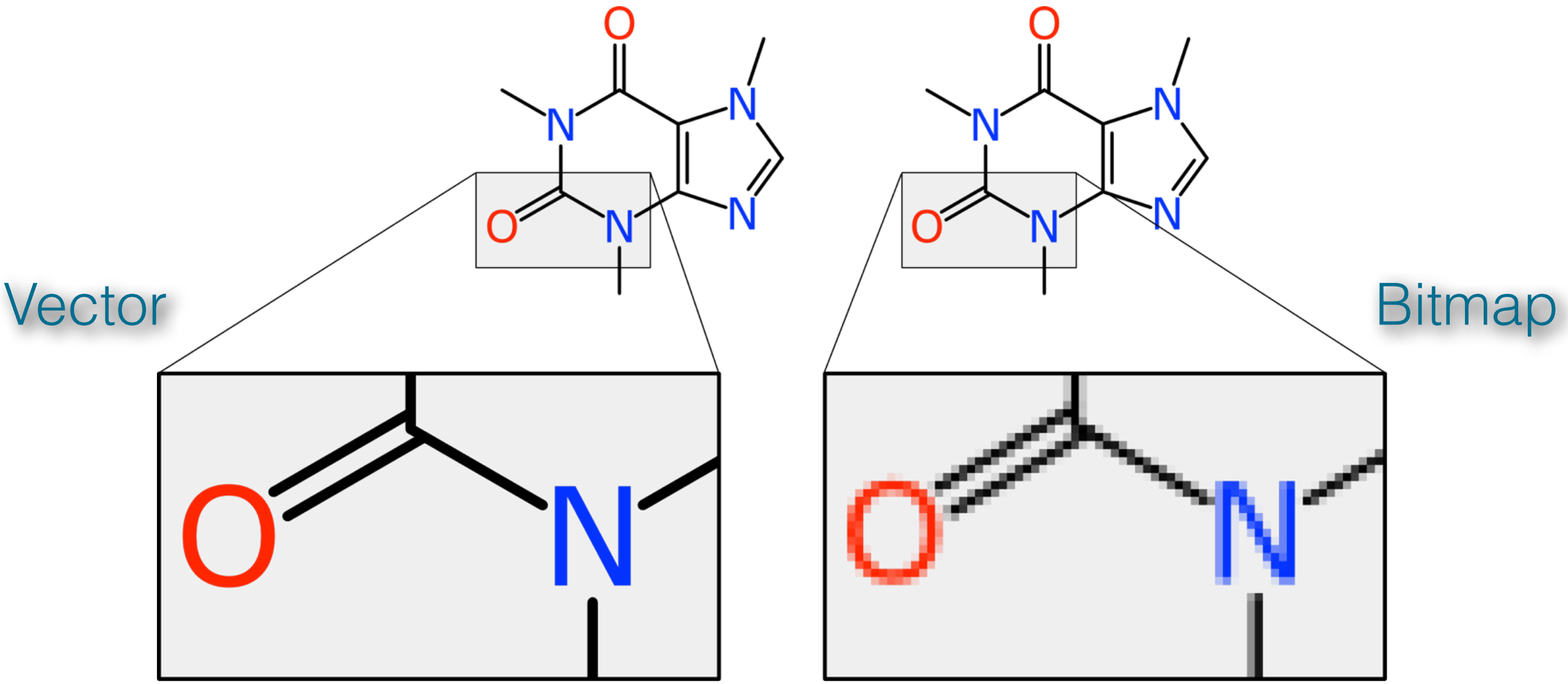


- Many ways to lookup molecular structure in online: e.g. Open with the *ChemSpider Mobile* app

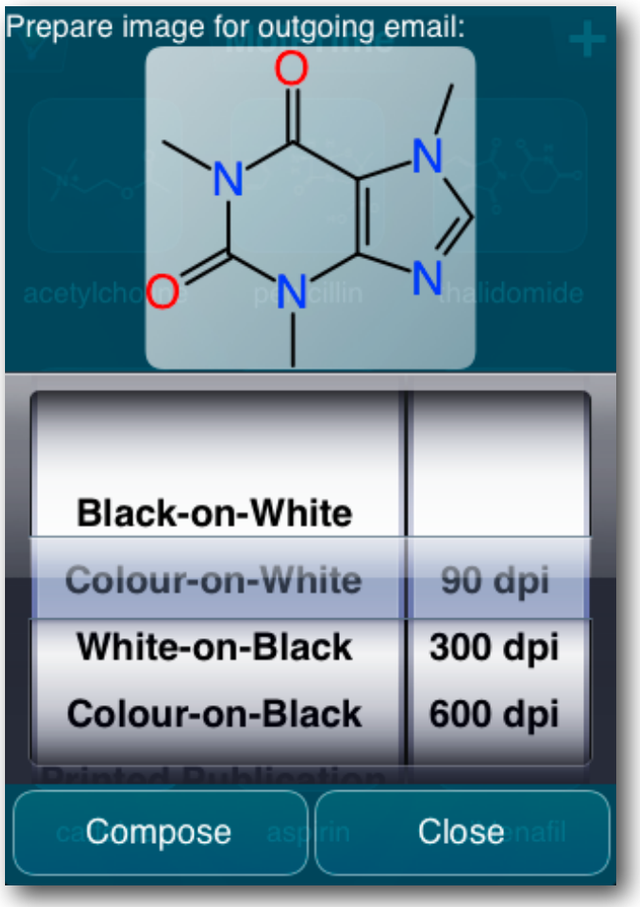
- Can also search *SPRESI*, *Mobile Reagents*, *PubChem*, *ChEBI*, *eMolecules*

Presentation

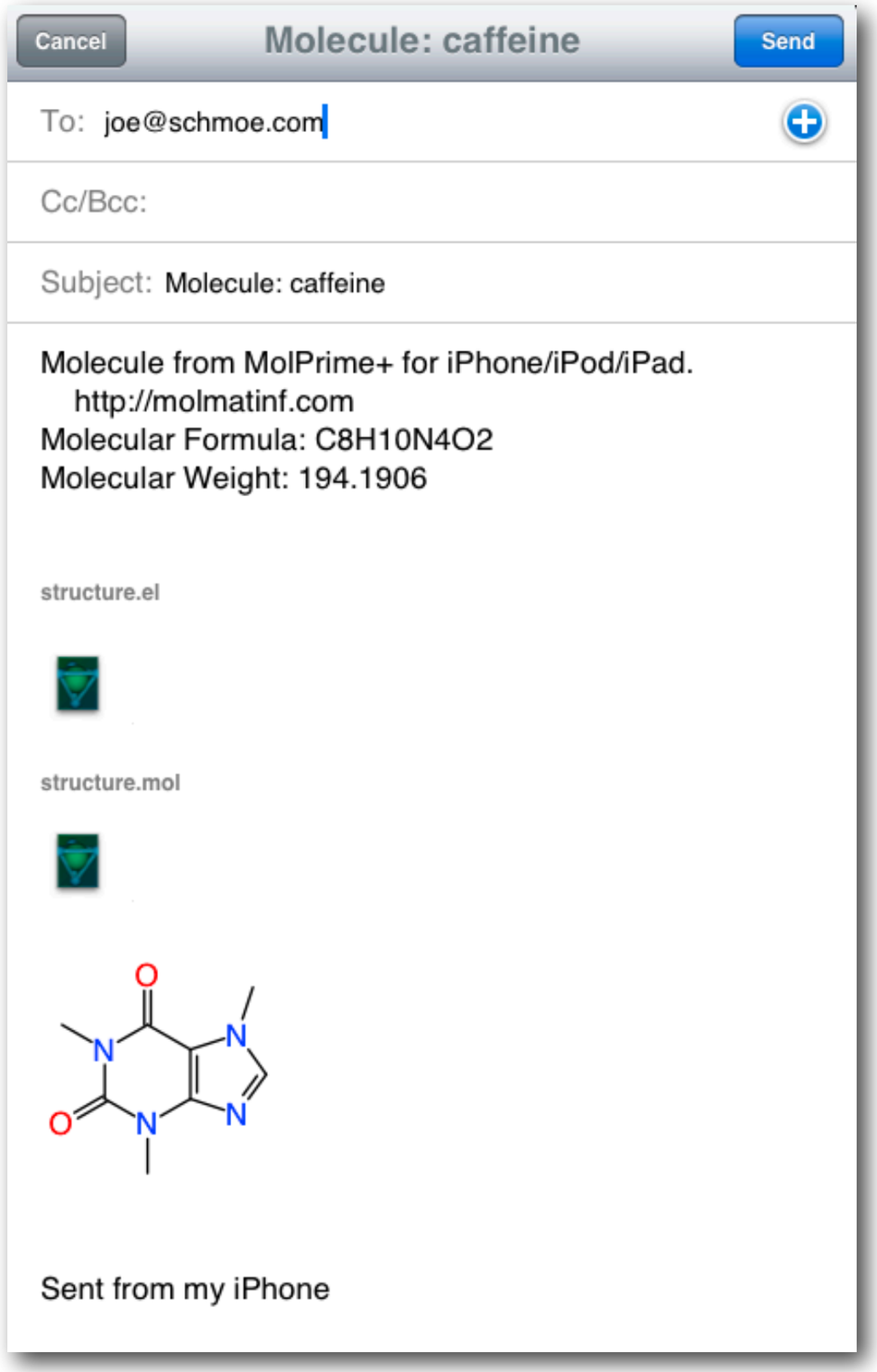
- Can copy bitmap to clipboard: paste into iWork
- Or create **vector graphics** (SVG, EPS, Word/Excel)



Sharing: Email



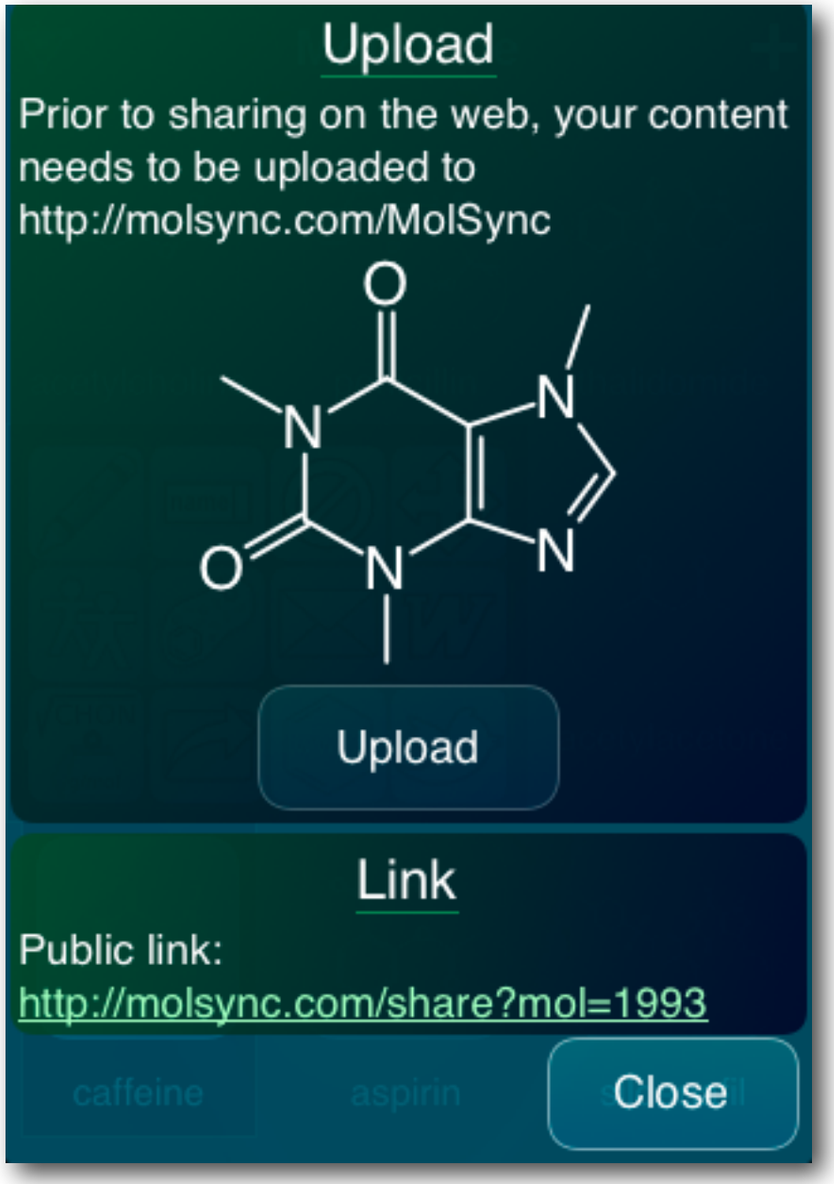
- Initiate an email, with an image, source data...



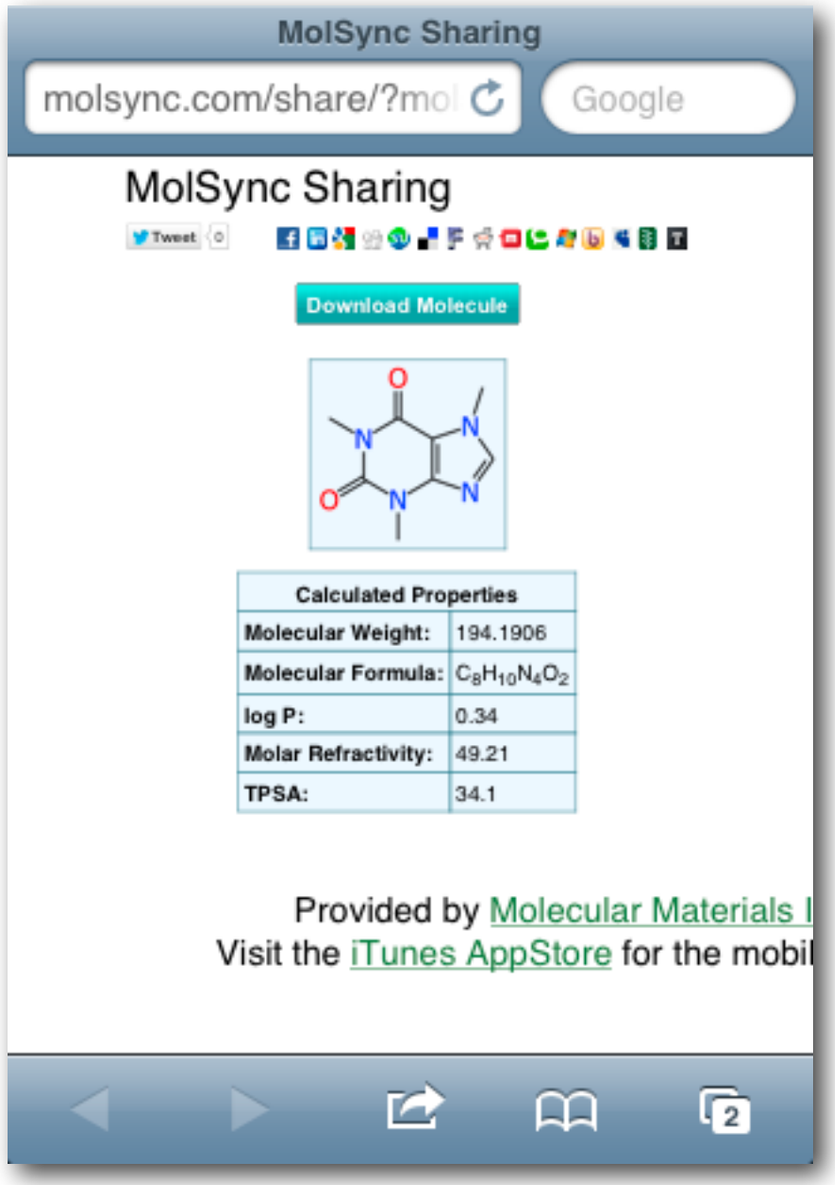
- Recipient can view the picture...

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

Sharing: Web

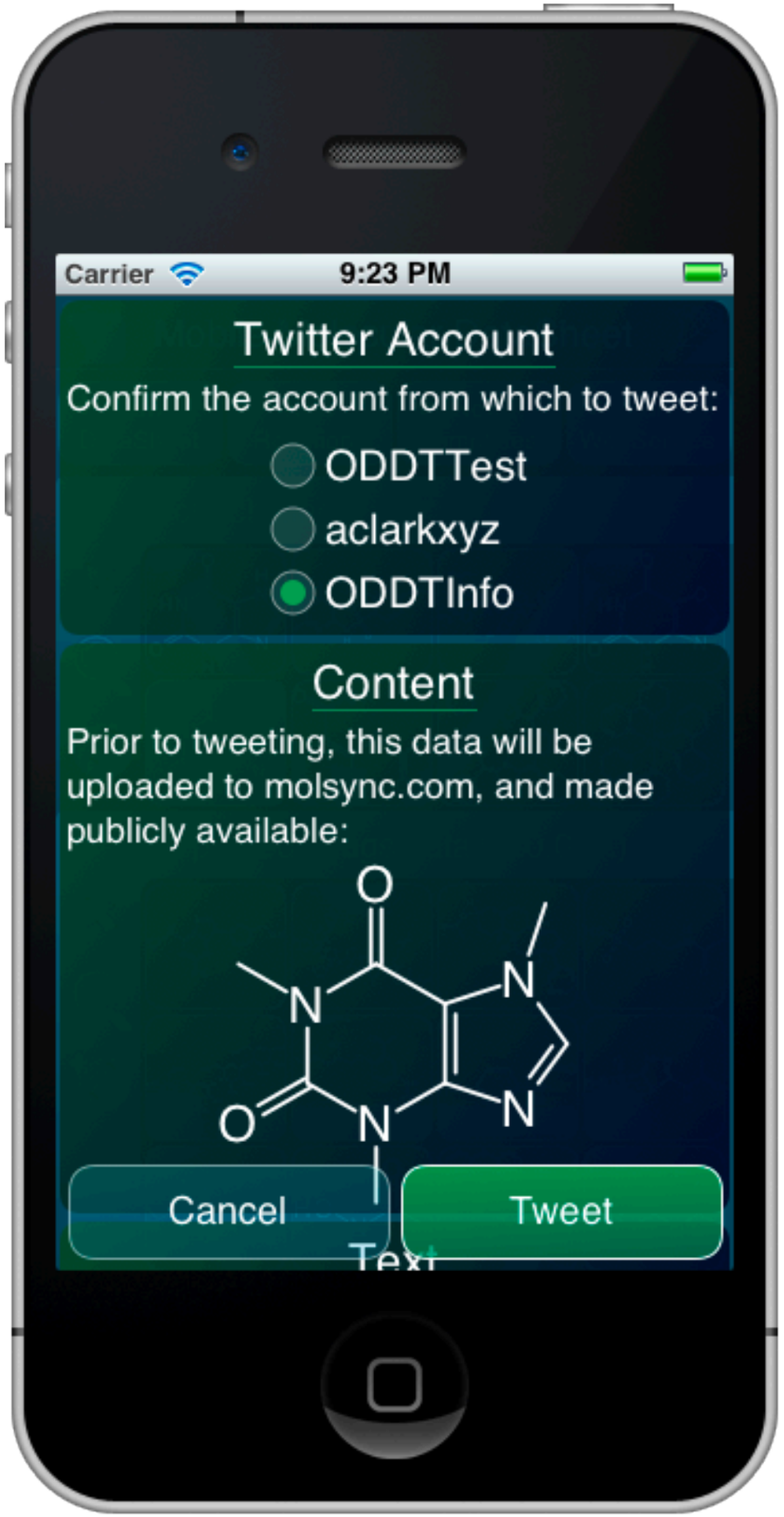


- Upload to **molsync.com**
- View public link



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

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

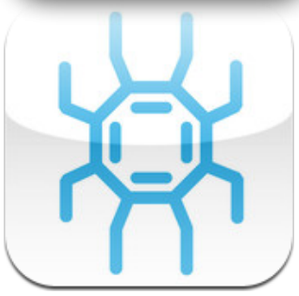
Green Solvents

Open Drug Discovery Teams (ODDT)

with *Collaborations in Chemistry*

ChemSpider Mobile

with *Royal Society of Chemistry*



SPRESI *mobile*

with *InfoChem*

Reaction101

with *Eidogen-Sertanty*

Yield101

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

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