

Chemistry in Your Pocket

*Shrinking cheminformatics applications
for mobile devices*

Dr. Alex M. Clark

Anaheim, March 2011

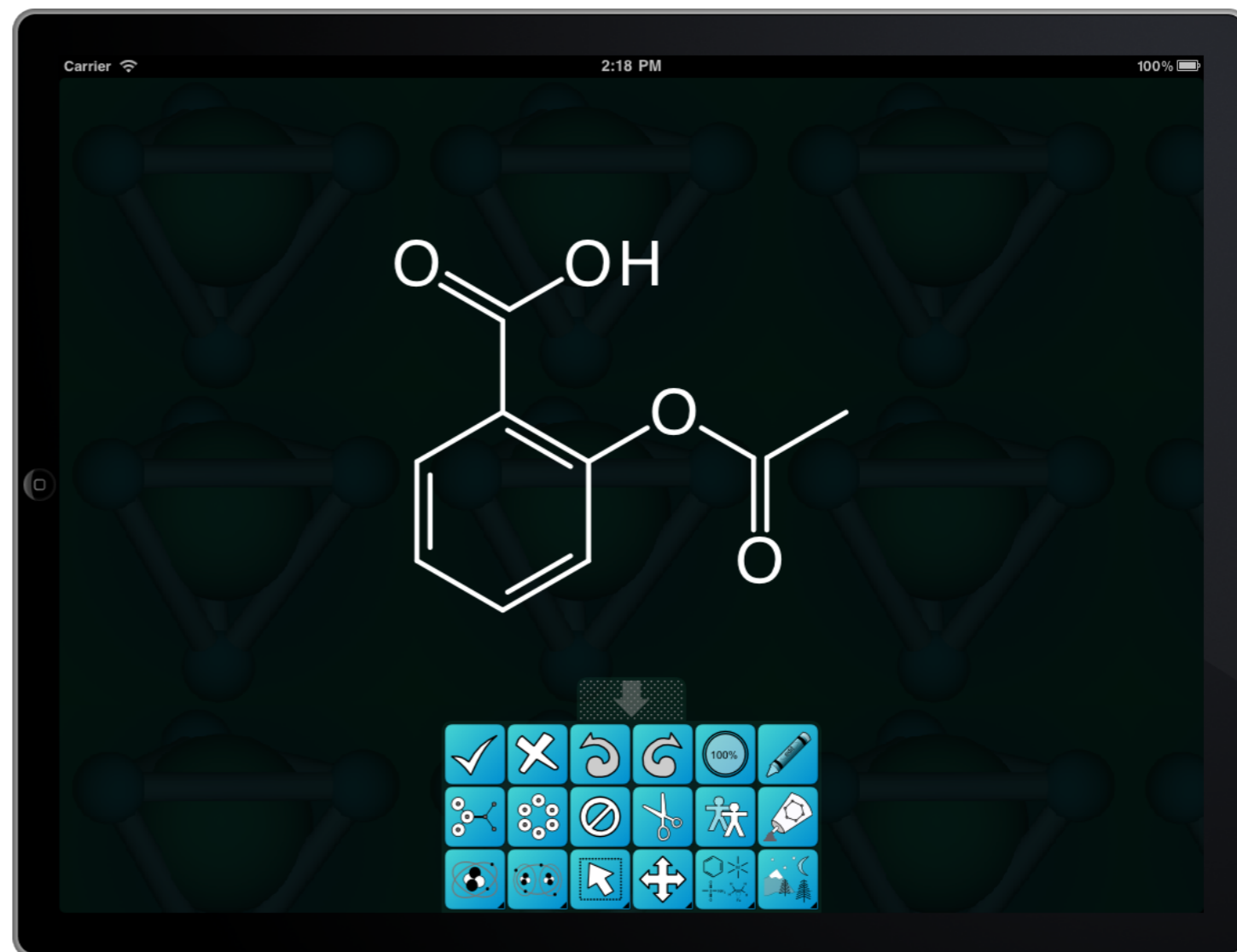


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<http://molmatinf.com>

Mobile Molecular DataSheet

Smartphones



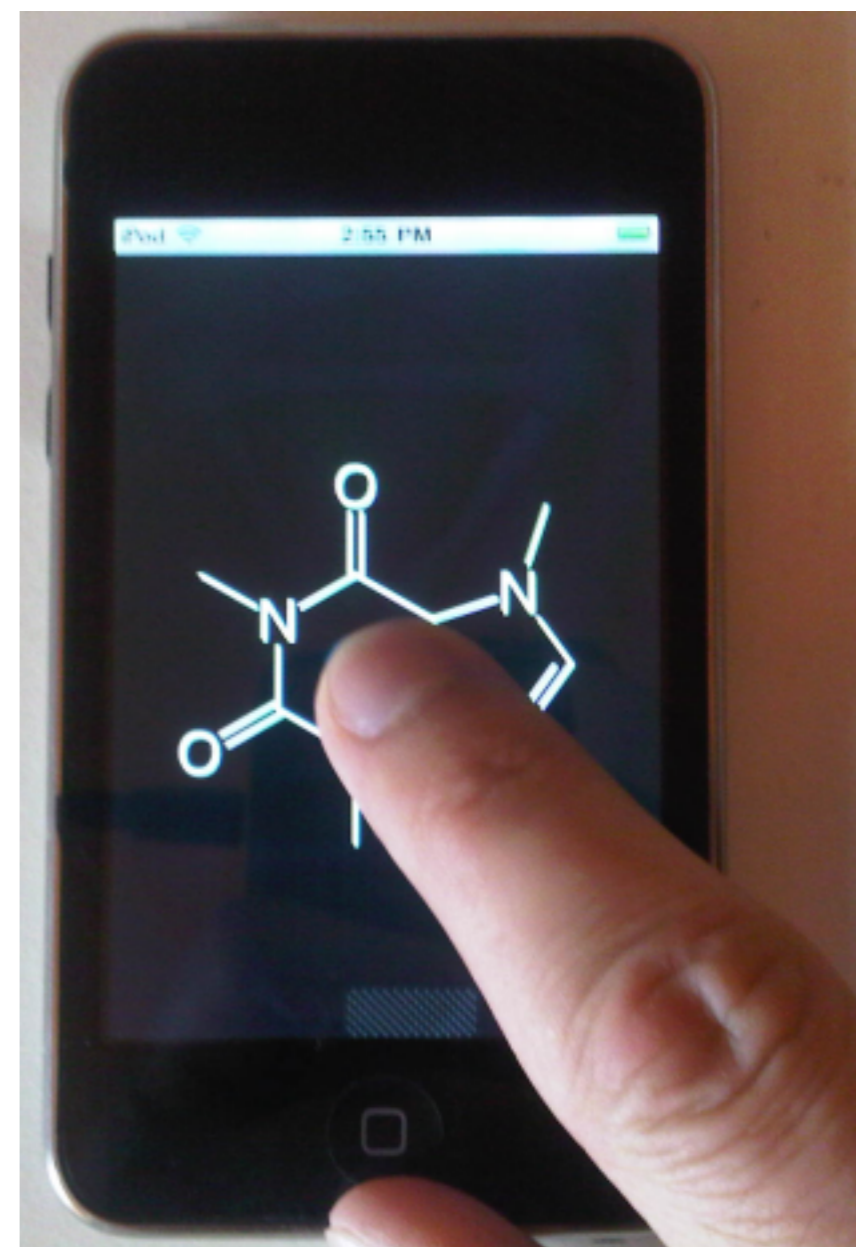
Tablets

Background

- Cheminformatics domain is desktop and server software... with a bit of web thrown in
- What about ultraportable devices?
- Smartphones and tablets powerful enough...
- ... but the user interface is very different.

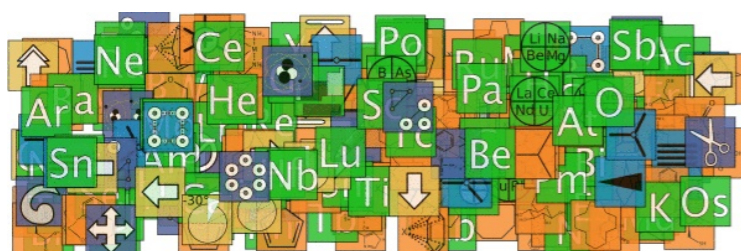
Sketcher challenges

- Many cheminformatics applications need the user to draw 2D structures
- Normal sketchers need a mouse
- A touchscreen is ***not*** the same!



Alternate approach

- Need a technique that does not require an accurate pointing device:



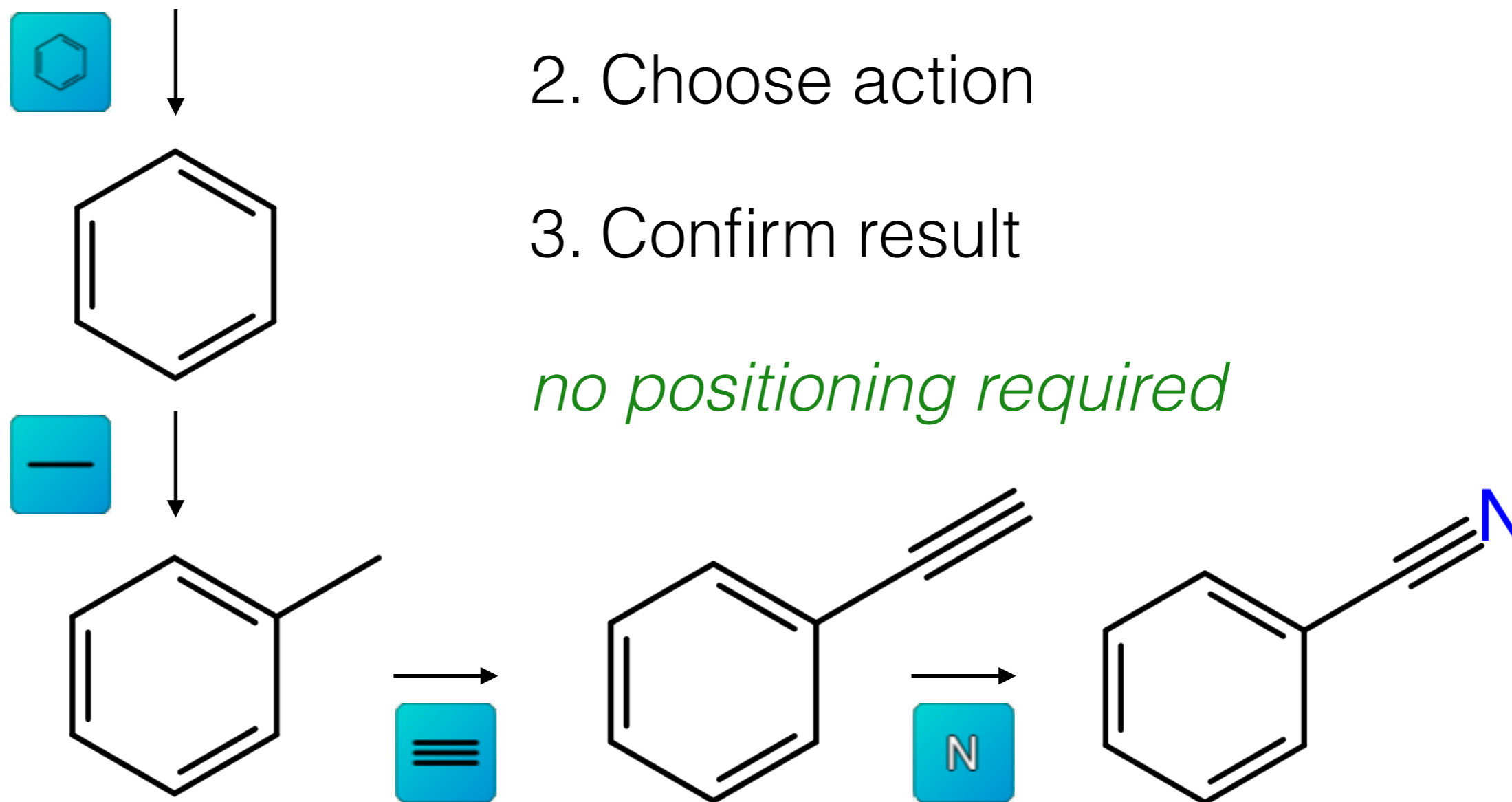
A.M. Clark, **Basic primitives for molecular diagram sketching**, *Journal of Cheminformatics* 2010, **2**:8.

- Sketching primitives maximise information content from limited user input, by inference and automation

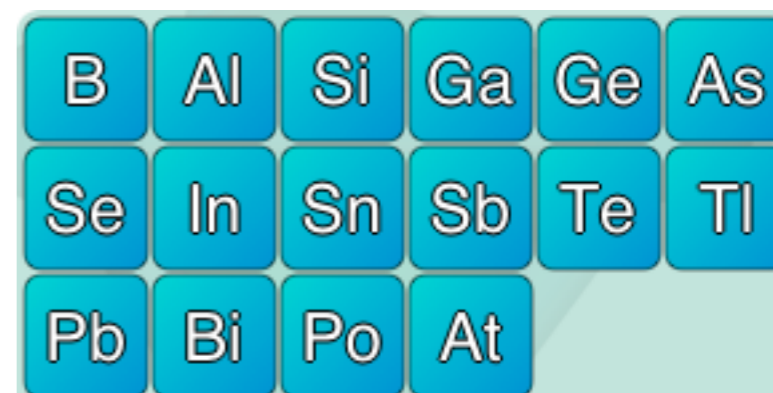
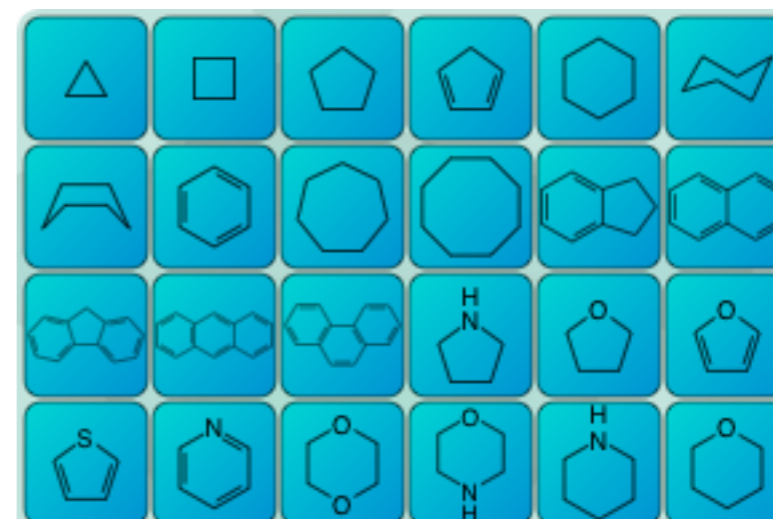
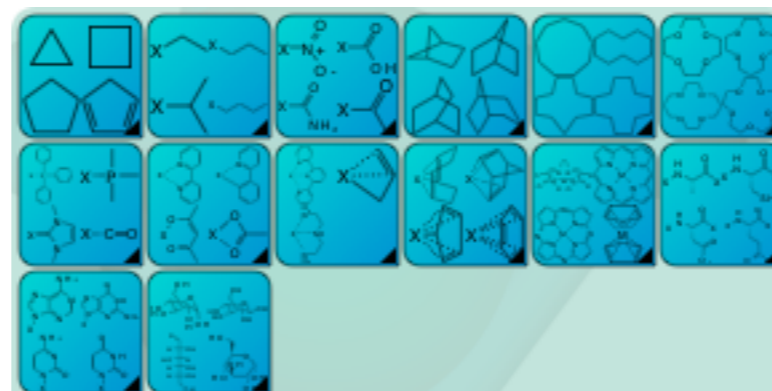
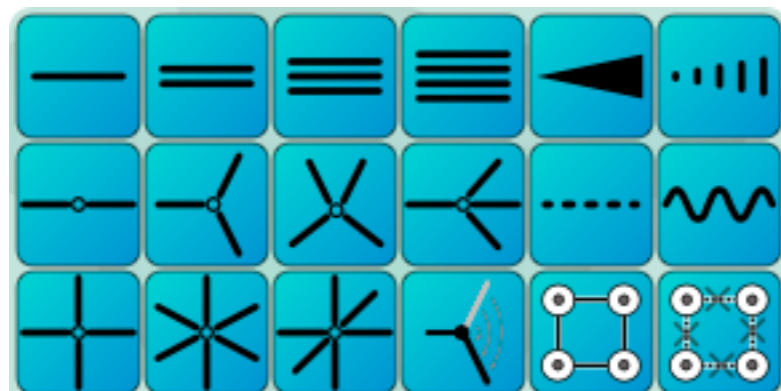
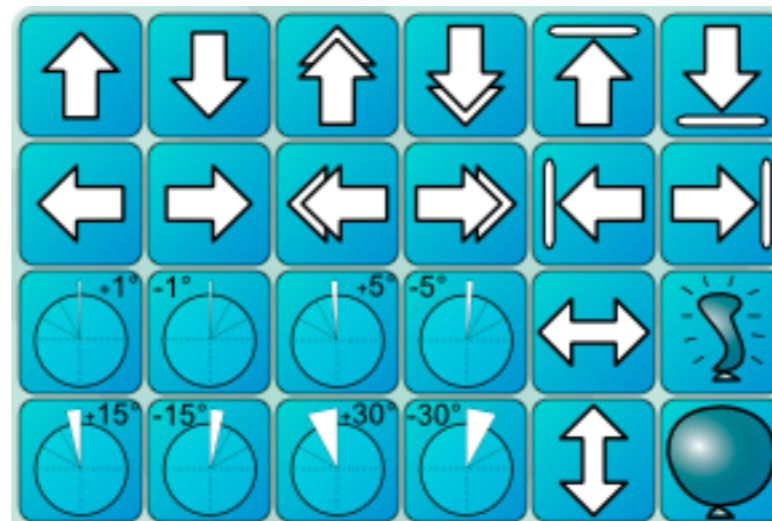
Sketching primitives

1. Pick atoms/bond
2. Choose action
3. Confirm result

no positioning required

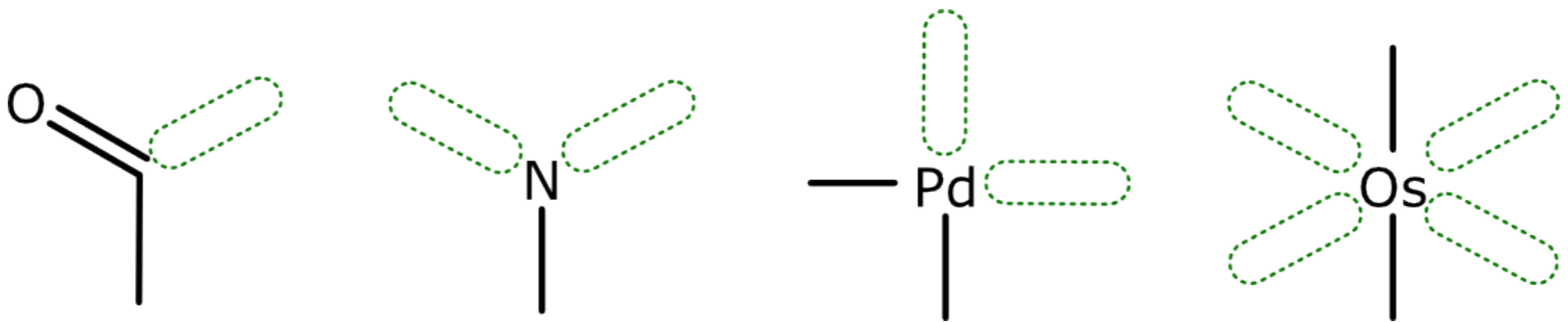


Primitives



Geometry

- Convenient sketching by guestimating geometry



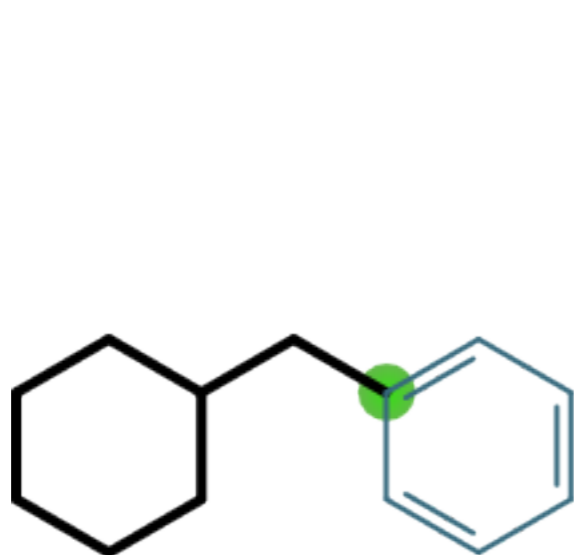
- Or specifying explicitly



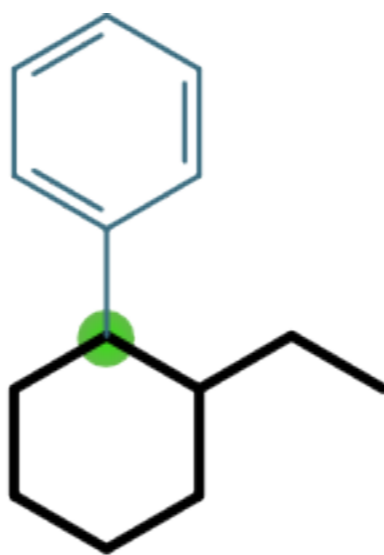
Templates

- Multiple fusion modes, multiple results

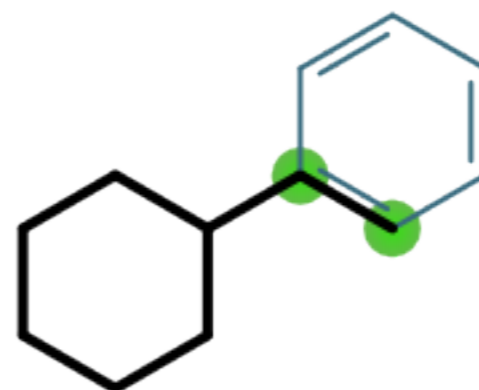
unguided



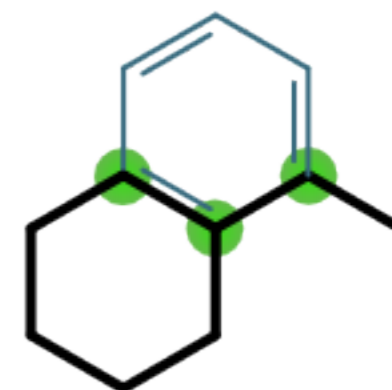
atom



bridge

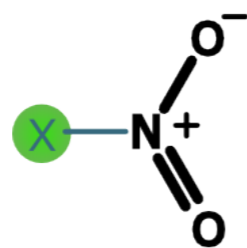


bond

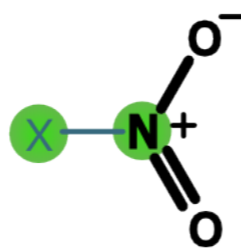


multi

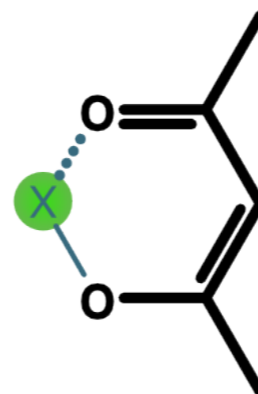
guided



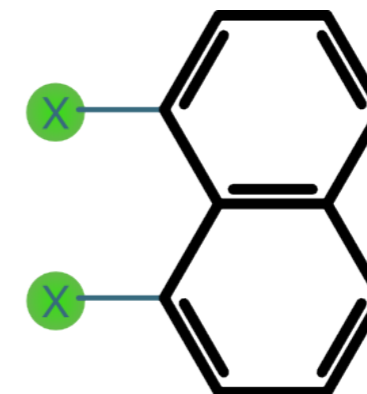
atom



bond

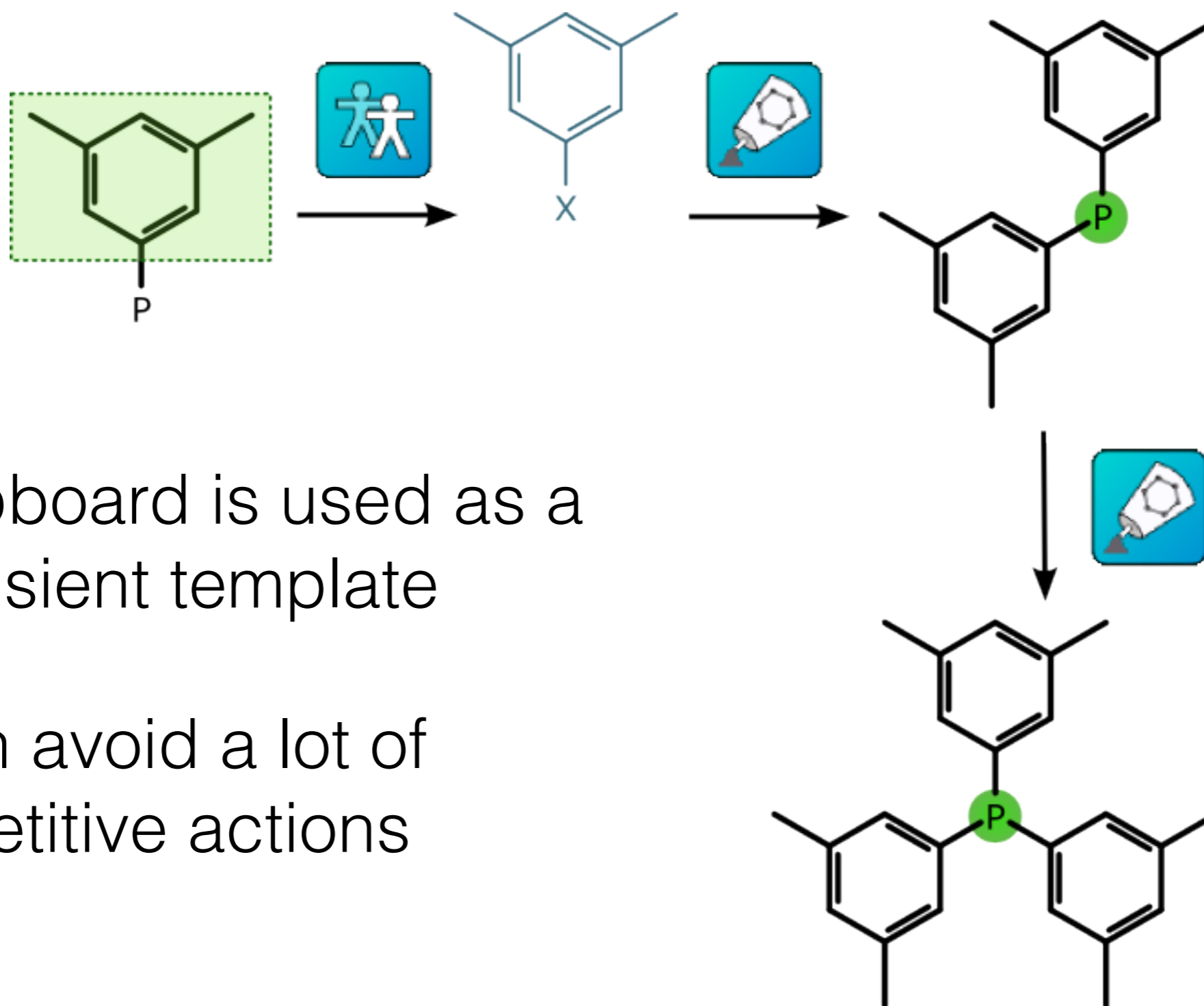


chelate



multi

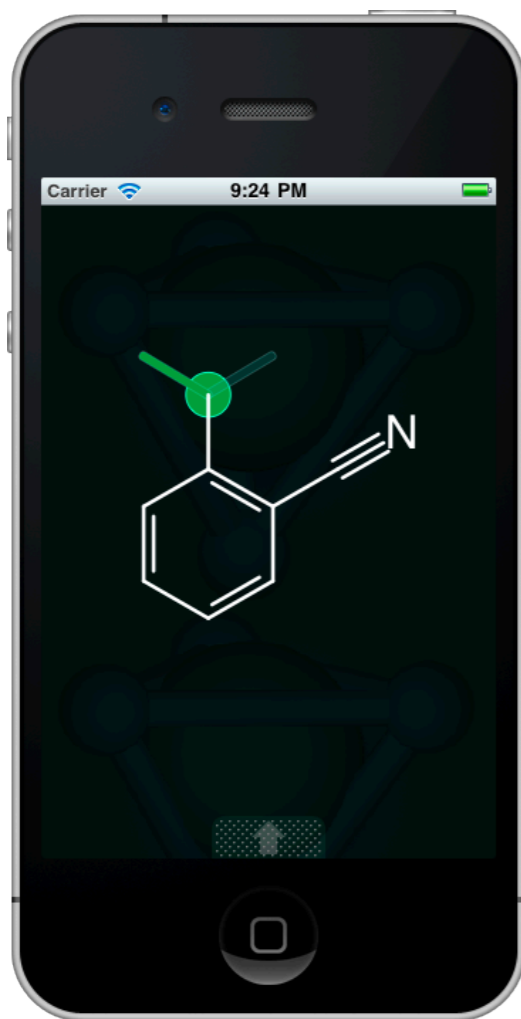
Clipboard



- Clipboard is used as a transient template
- Can avoid a lot of repetitive actions

Gestures

- Primitives only require very limited input, e.g. trackpad... touchscreens can do more:



Finger drawing








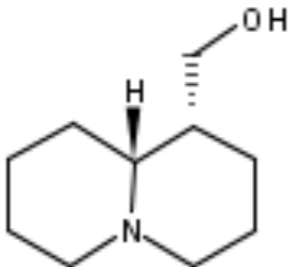
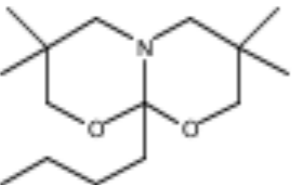
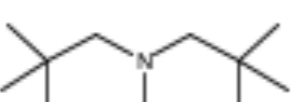
Crayon selection



Context menus

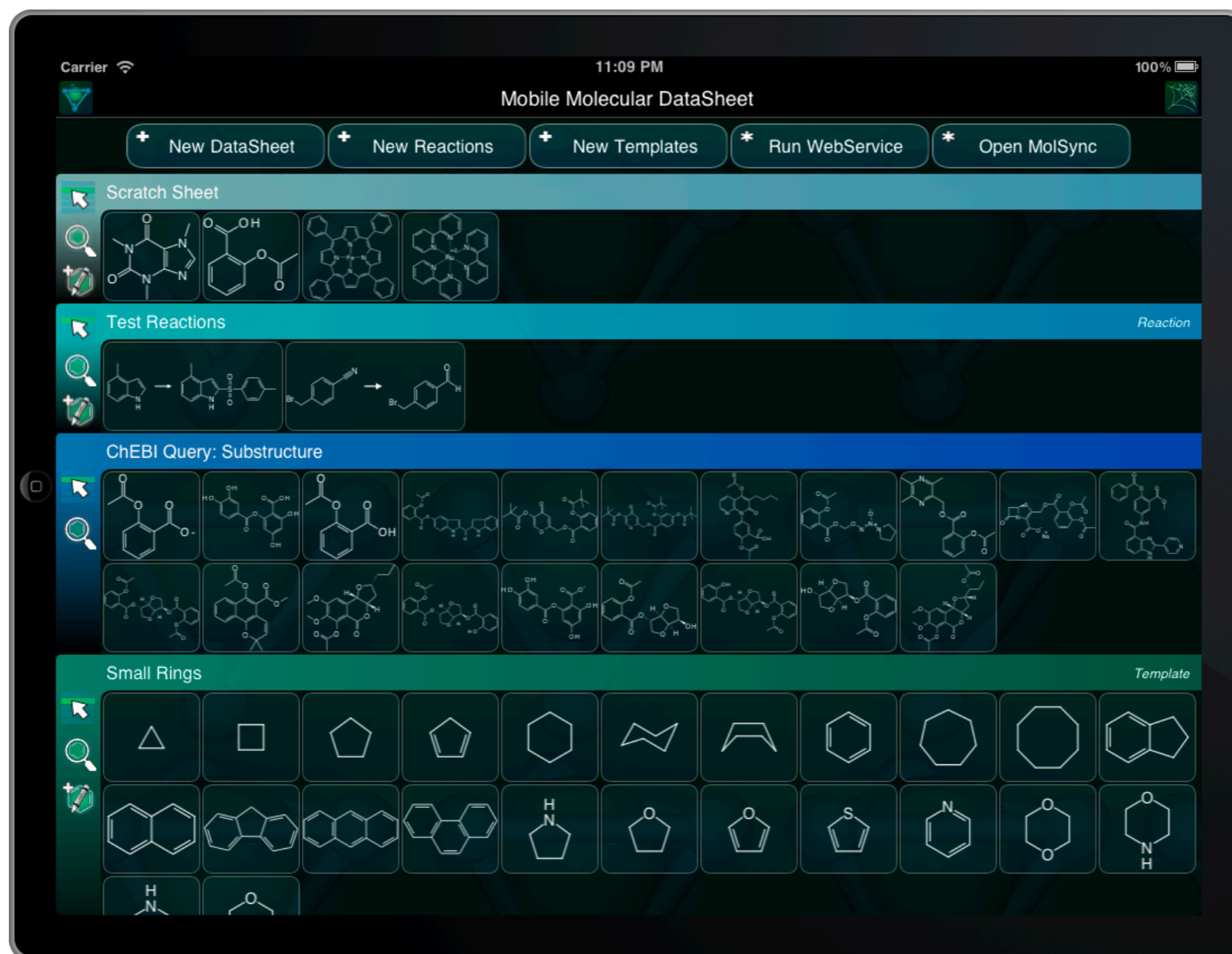
Now what?

- Have a sketcher that can draw publication quality diagrams quickly...
- ... next step is to group molecules and data together into "DataSheets":

	Molecule 	Name 	Formula 	MW 	R 
1		lupinine	C ₁₀ H ₁₉ NO	169.264	
2		8a-butyl-3,3,6,6-tetramethyltetra	C ₁₅ H ₂₉ N ₀₂	255.3963	
3		3,3,6,6,8a-pentamethyltetrahydro	C ₁₂ H ₂₃ N ₀₂	213.31656	

Directory of DataSheets

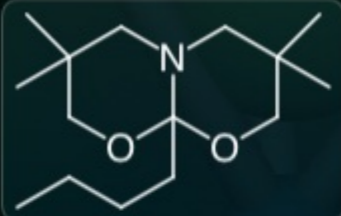
- Represent each row with a molecule glyph:



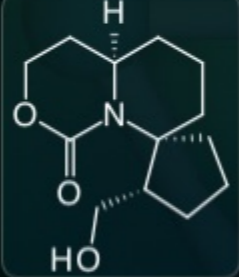
Detail view

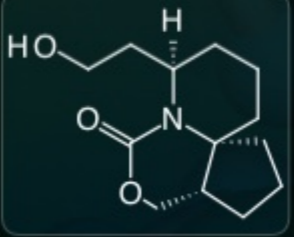
iPad 12:00 AM 100%

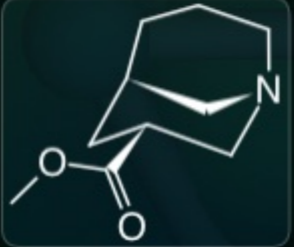

Name: lupinine
Formula: C₁₀H₁₉NO
MW: 169.264


Name: 8a-butyl-3,3,6,6-tetramethyltetrahydro-1,8-dioxo-4a-azanaphthalene
Formula: C₁₅H₂₉NO₂
MW: 255.396


Name: 3,3,6,6,8a-pentamethyltetrahydro-1,8-dioxo-4a-azanaphthalene
Formula: C₁₂H₂₃NO₂
MW: 213.317


Name: (1S,2S,4a'R)-2-(hydroxymethyl)hexahydrospiro[cyclopentane-1,8'-pyrido[1,2-c][1,3]oxazin]-1'-one
Formula: C₁₃H₂₁NO₃
MW: 239.311

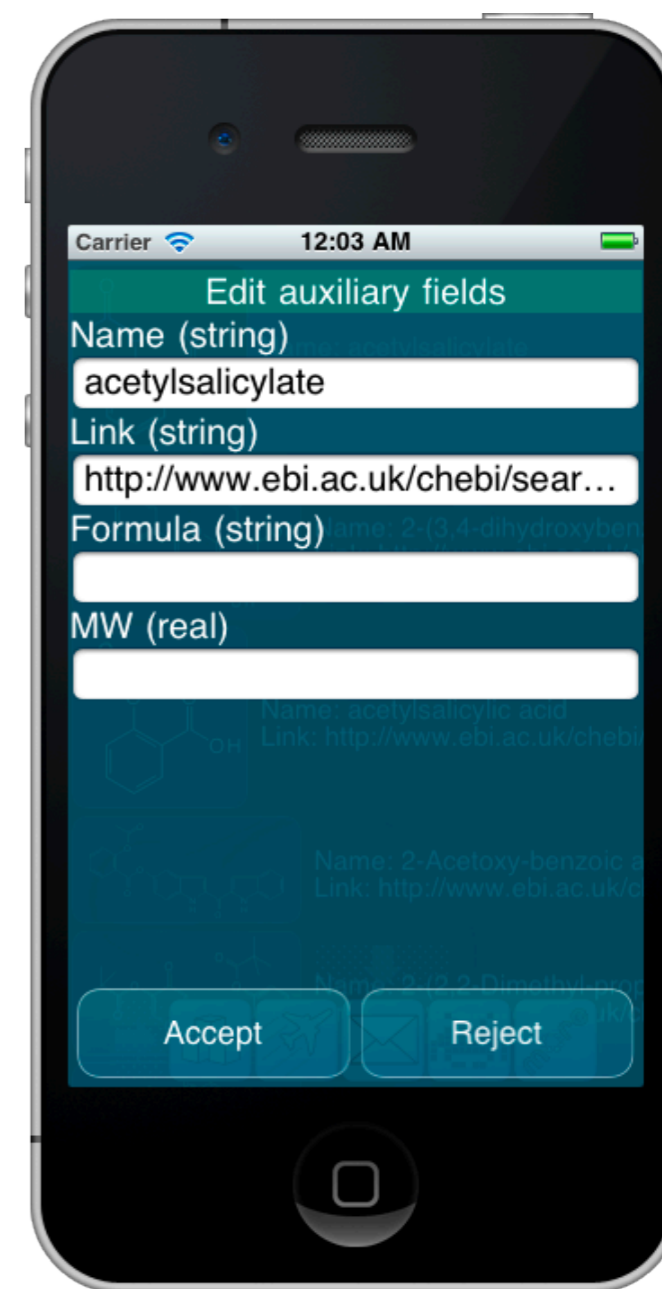
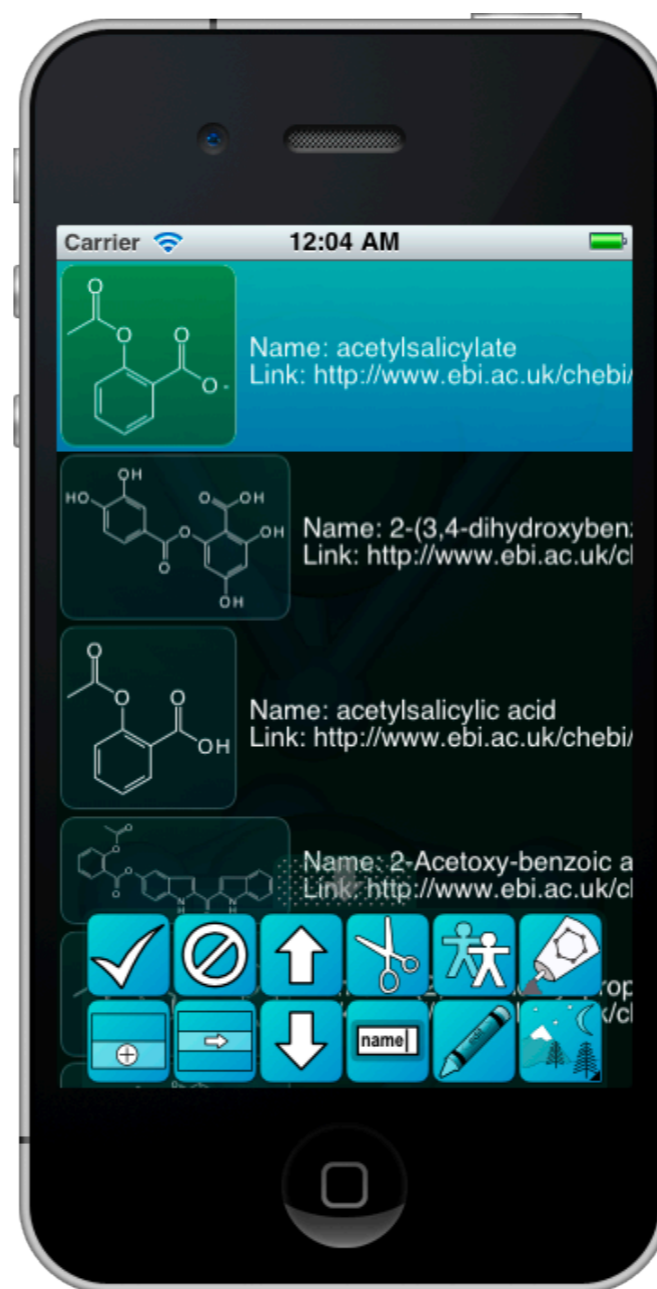

Name: (3aS,7R,10aS)-7-(2-Hydroxy-ethyl)-octahydro-5-oxa-6a-aza-cyclopenta[d]naphthalen-6-one


Name: 1-Aza-bicyclo[3.3.1]nonane

Navigation icons: ✓, ✗, ↑, ✂, 👤, 📄, 📄, ⇌, ↓, name|, 🖋️, 🌄

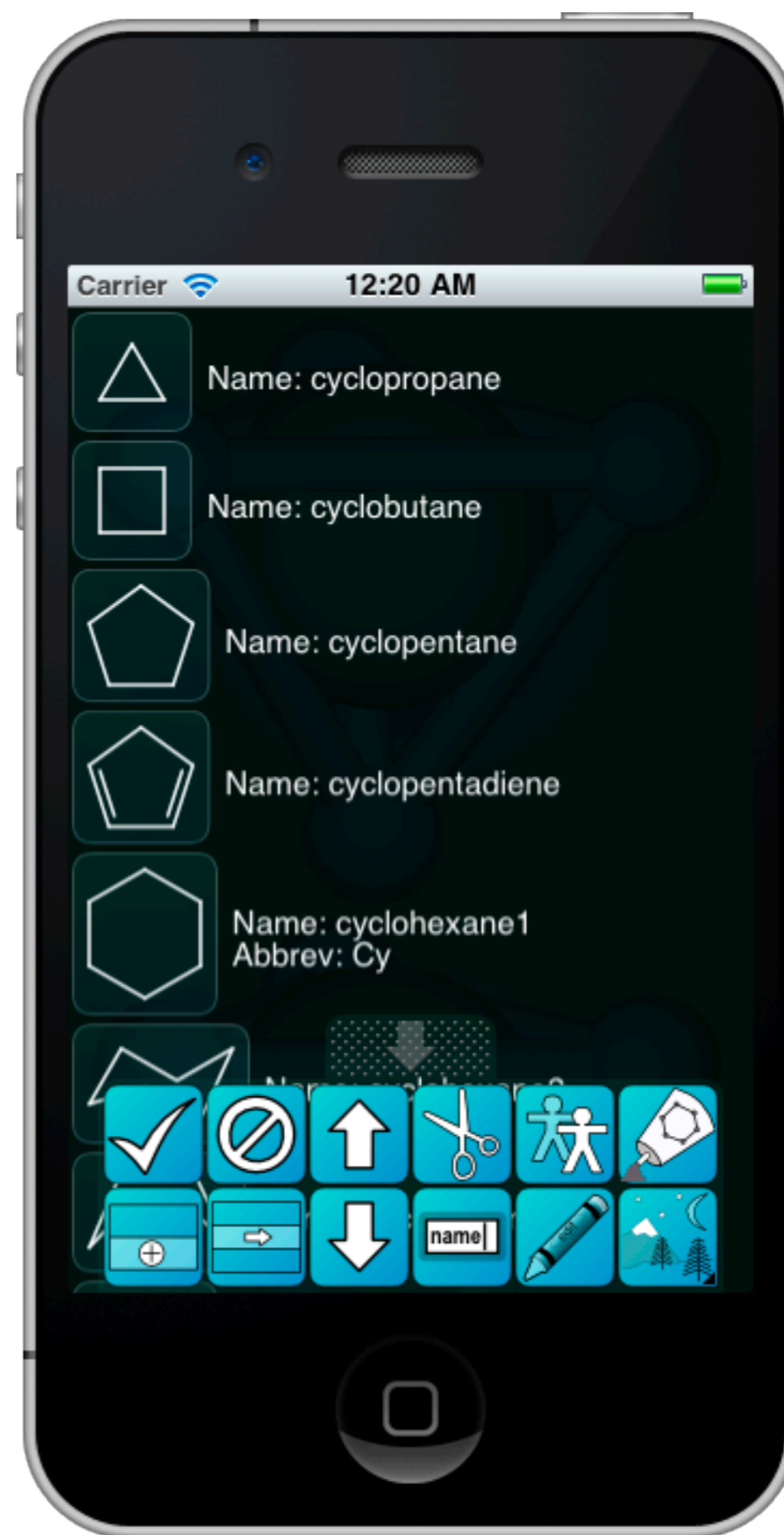
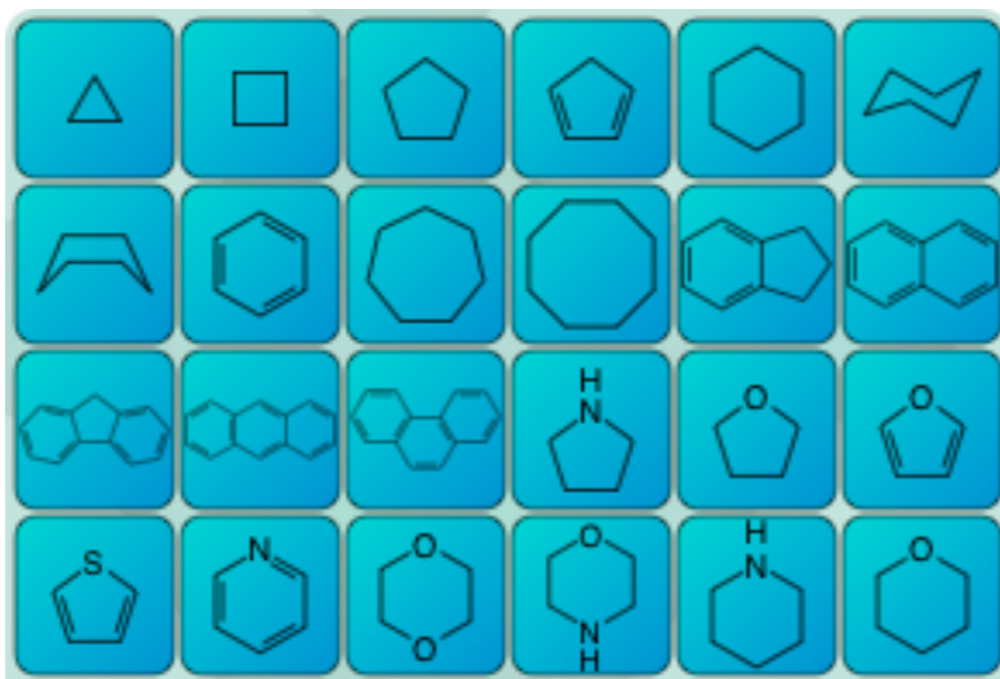
Editing

- Edit structures, scalar fields, table structure, etc.
- Each task uses a full screen panel



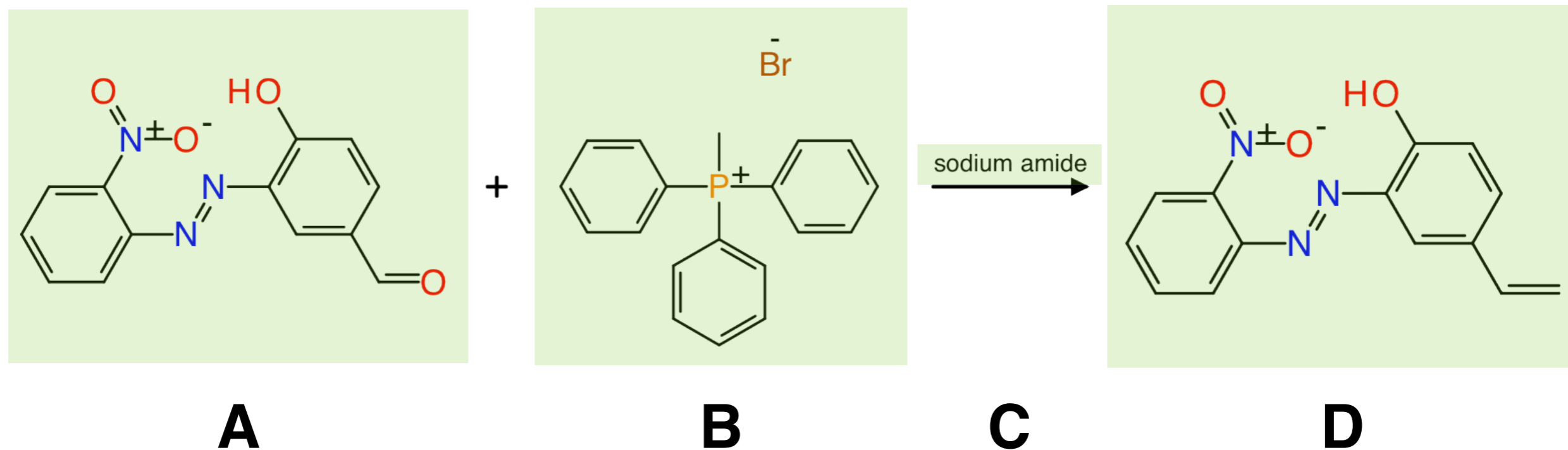
Templates

- Just like normal datasheets
- Their content is used to compose the template groups:

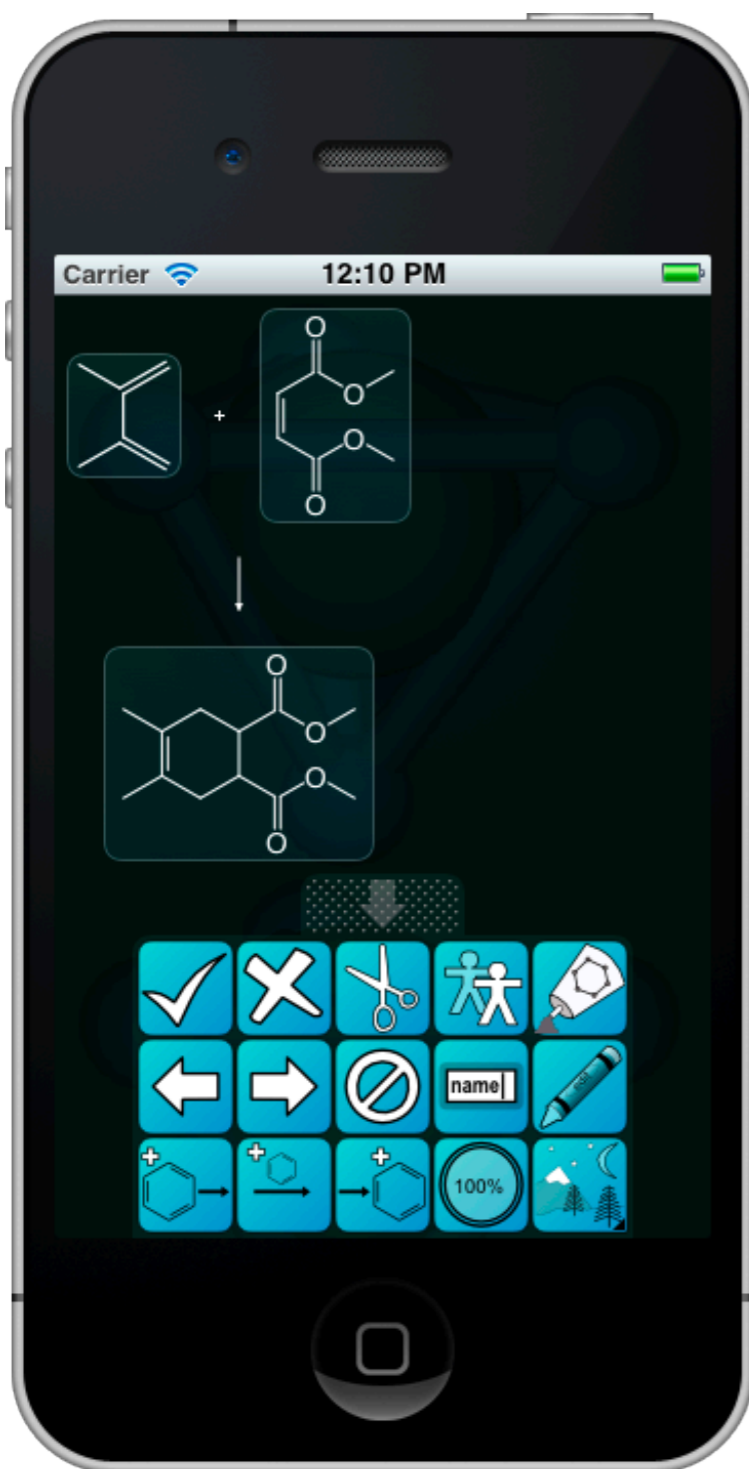


Reactions

- Devices too small for "freeform" editing, but separate components is viable:



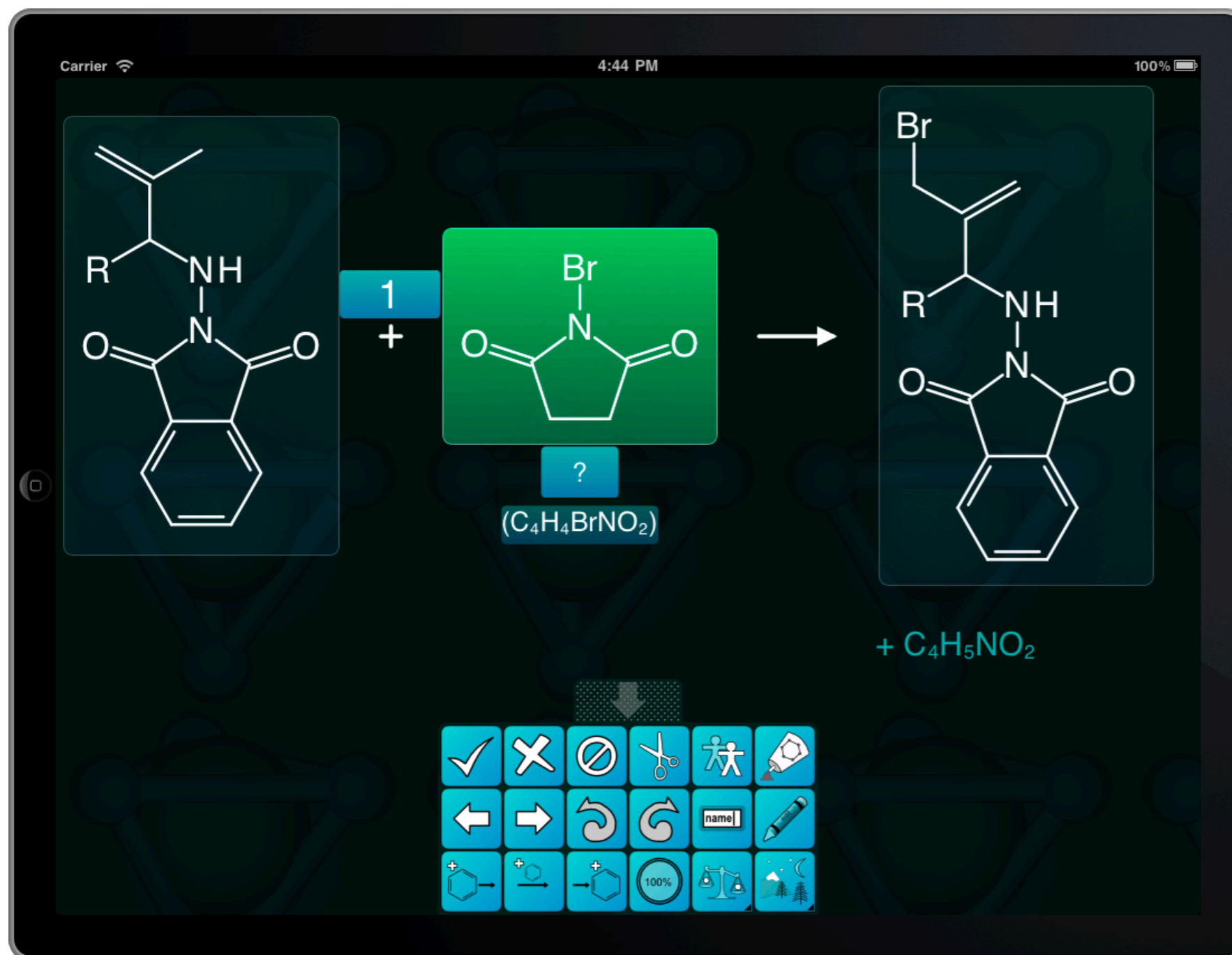
Reaction editing



- Dedicated editor
- Stored as one row per reaction
- ELN friendly format

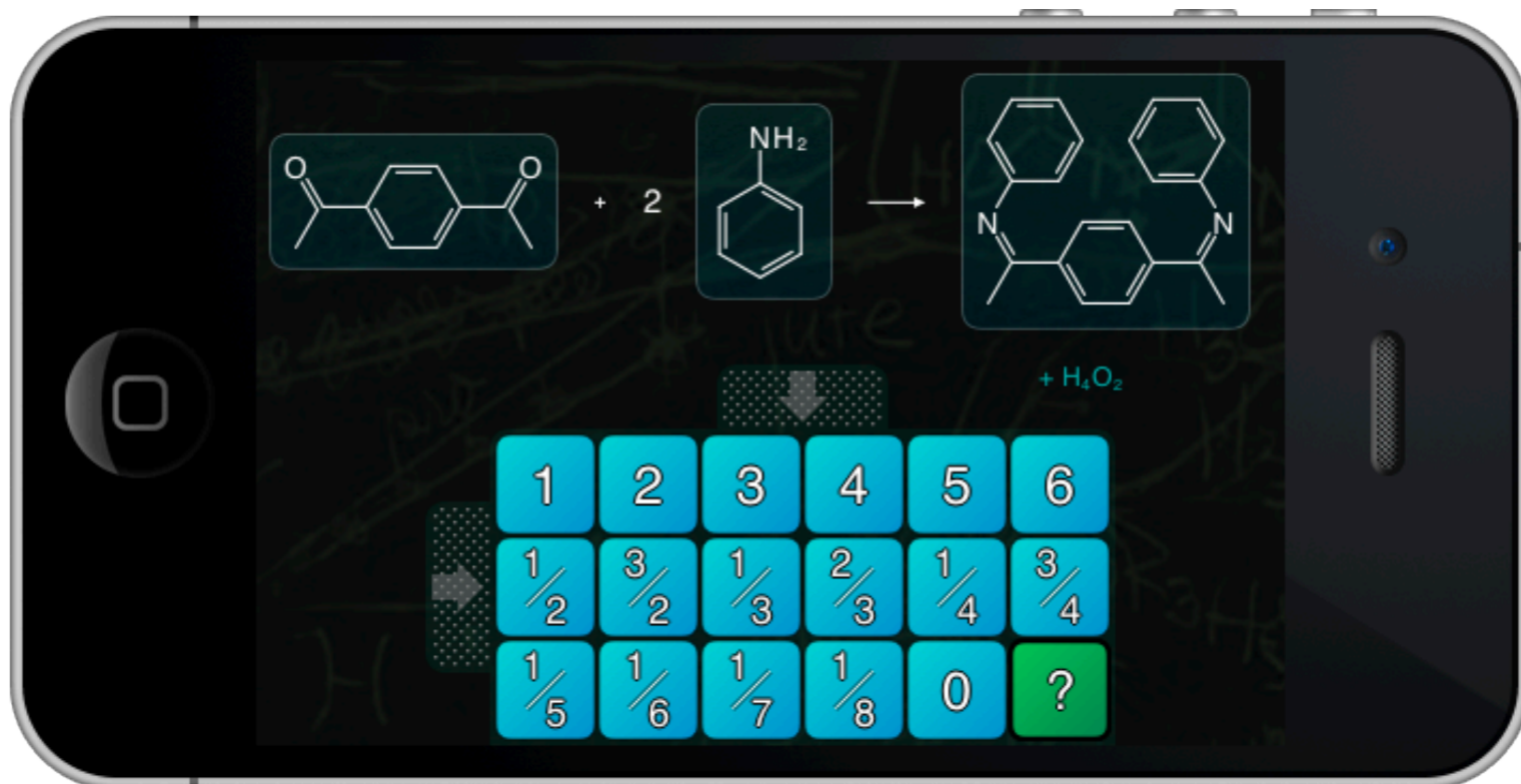
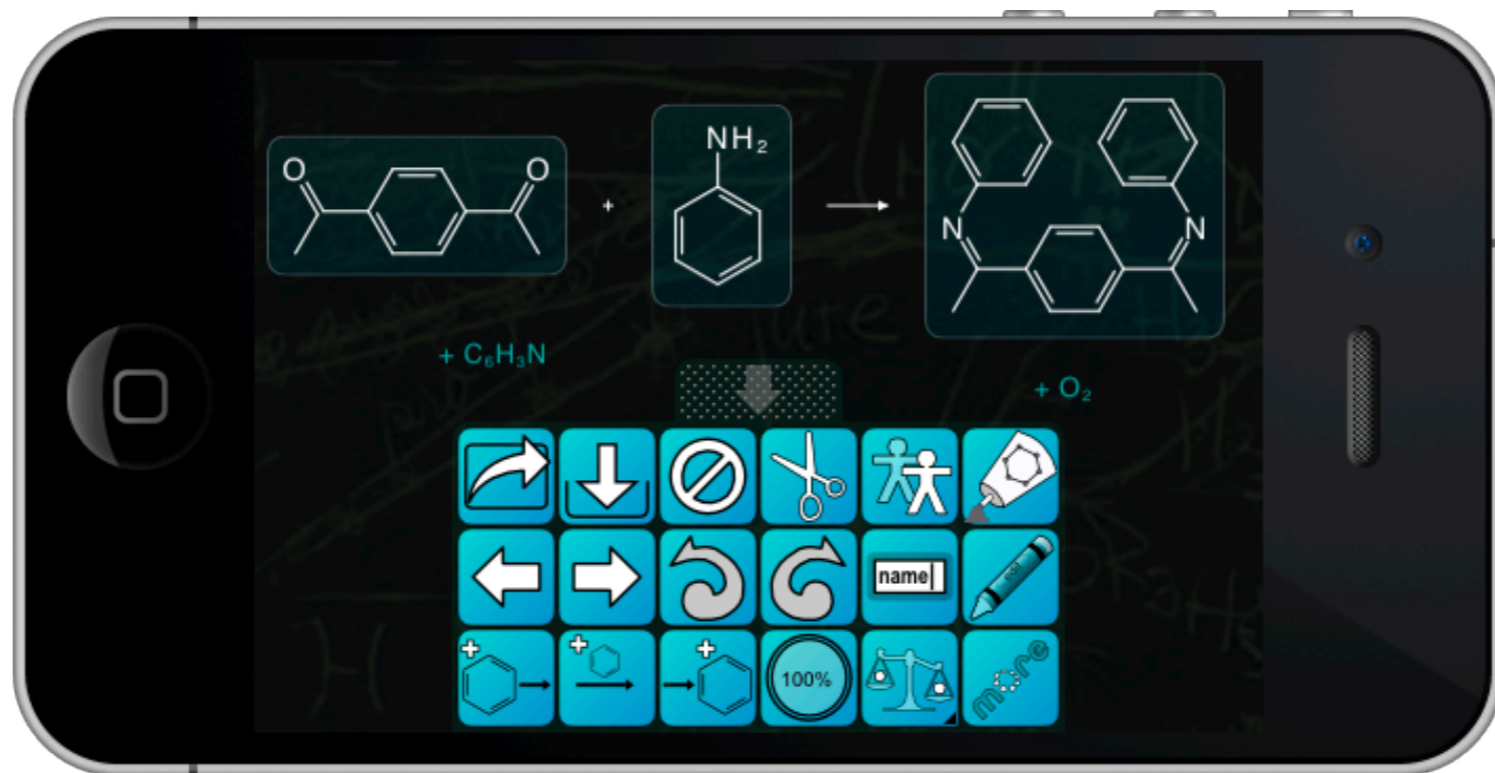


On tablets



- Landscape on iPad is ideal

Stoichiometry

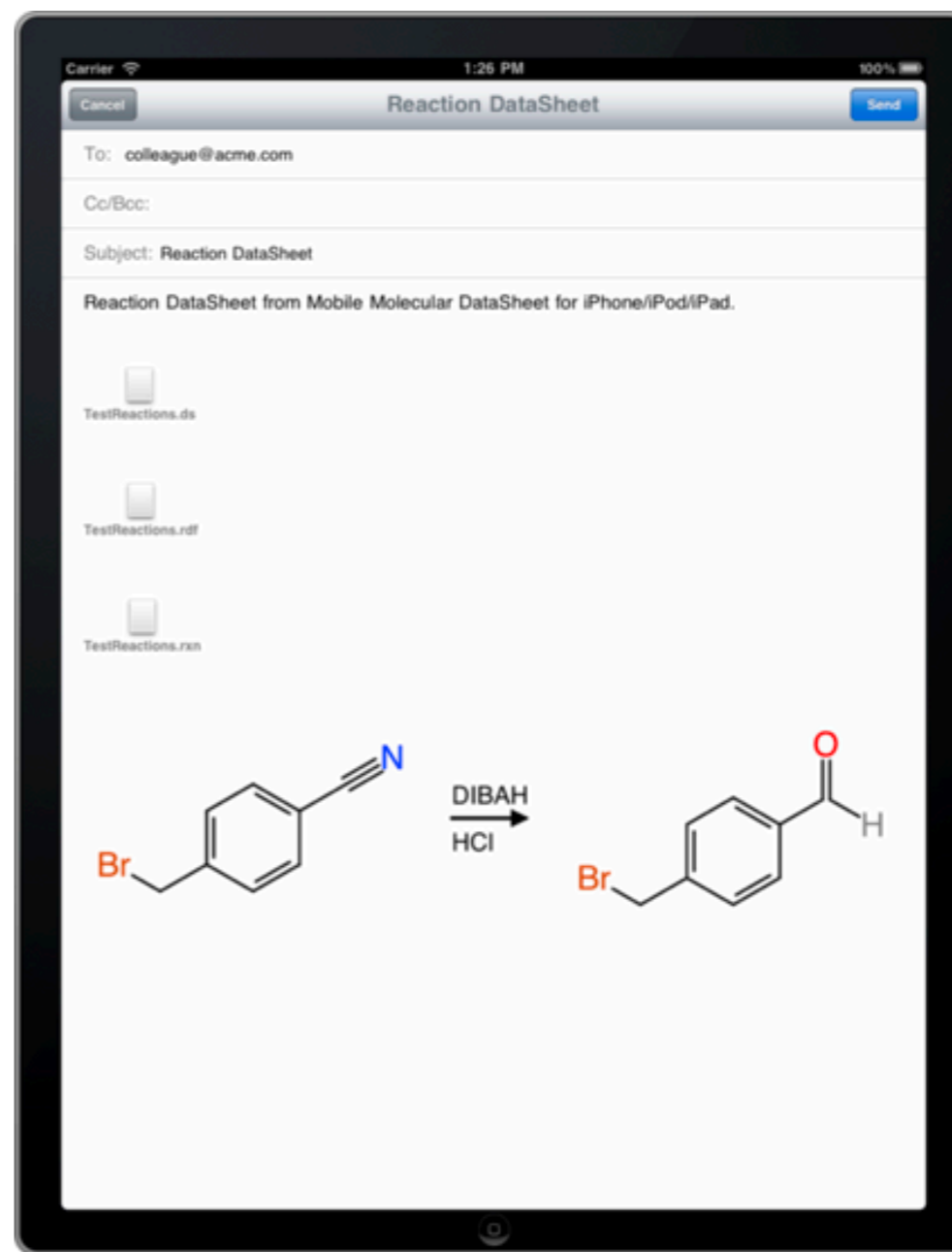
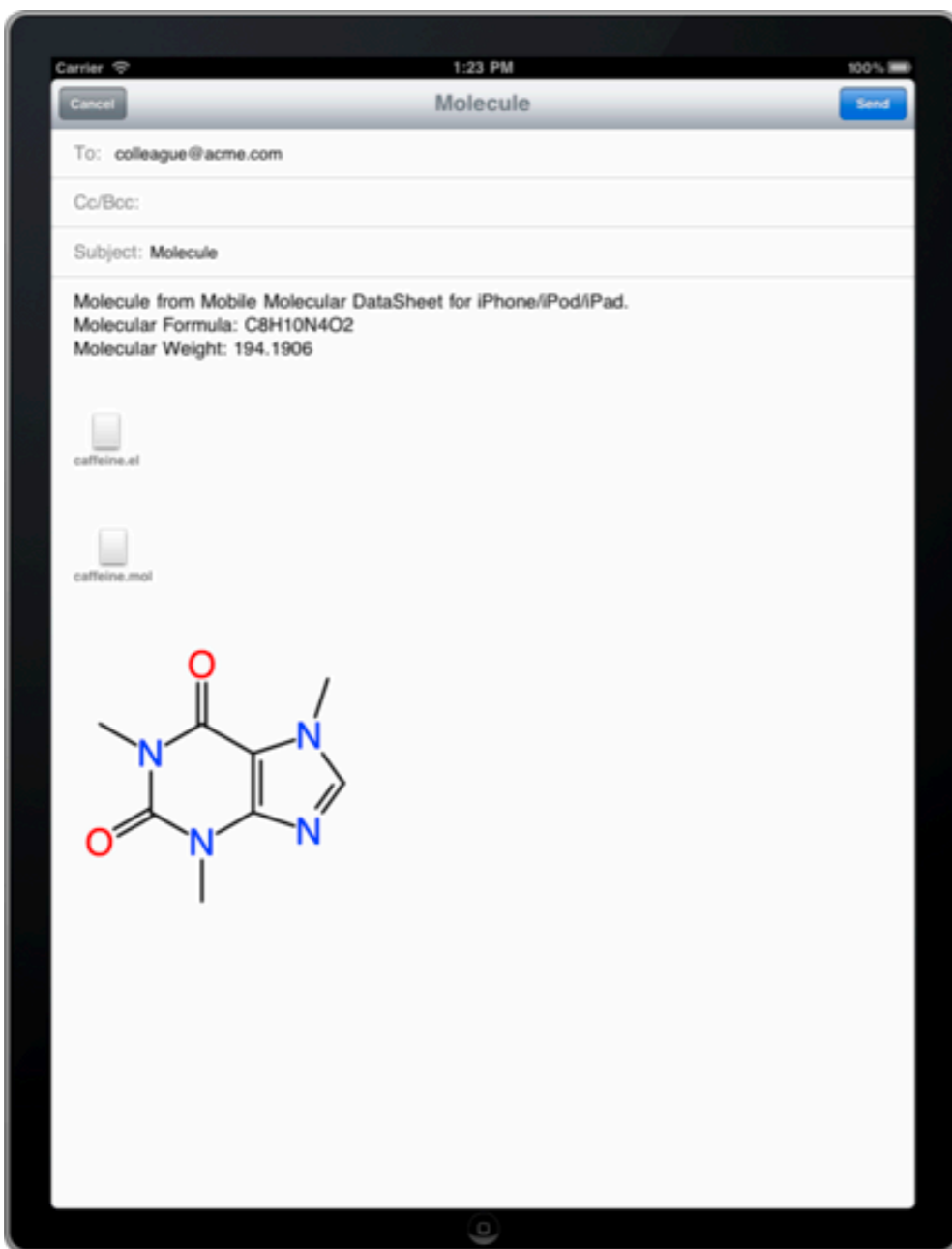


Communication

- Editing and arranging data doesn't happen in isolation
- Mobile apps typically have access to:
 - Email attachments
 - HTTP connections
 - File transfer by cable
 - Other installed apps

Sending email

- Include chemical data and an image:



Receiving email

- Attachments include industry standard formats (MDL), file extensions and MIME types
- Exchange data with other mobile users, or the outside world
- Opens directly into app...

iPad 1:44 PM 100%

Inbox 1 of 50


From: Alex Clark Hide


To: aclark.xyz@gmail.com

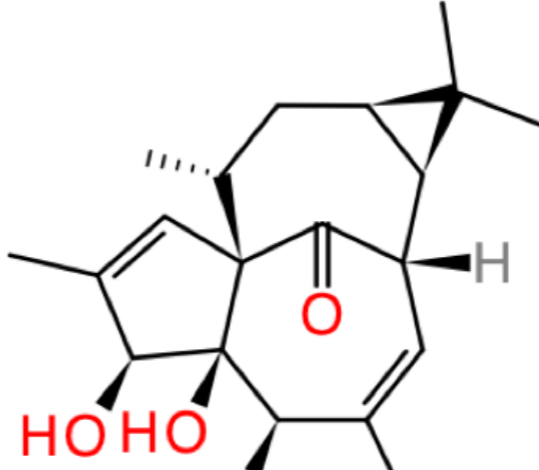
Molecule

5 March, 2011 1:42 PM [Mark as Unread](#)

Molecule from Mobile Molecular DataSheet for iPhone/iPod/iPad.
Molecular Formula: C₂₀H₂₈O₅
Molecular Weight: [348.4333](#)

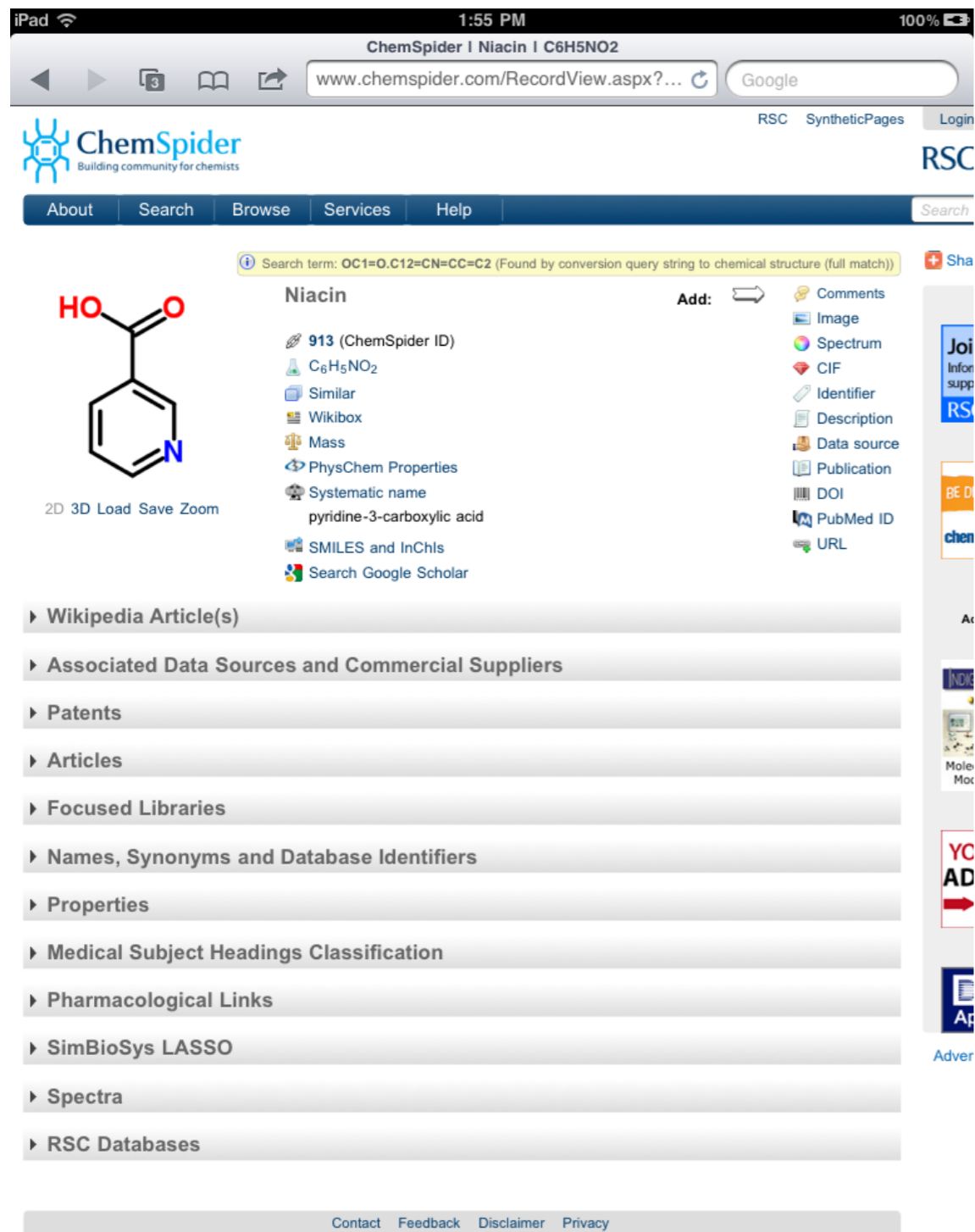
 0.9 KB **Open in "MMDS"**

 2.6 KB



Web downloads

- Same mechanism as attachments...



ChemSpider | Niacin | C₆H₅NO₂

www.chemspider.com/RecordView.aspx?...

ChemSpider Building community for chemists

Search term: OC1=O.C12=CN=CC=C2 (Found by conversion query string to chemical structure (full match))

Niacin

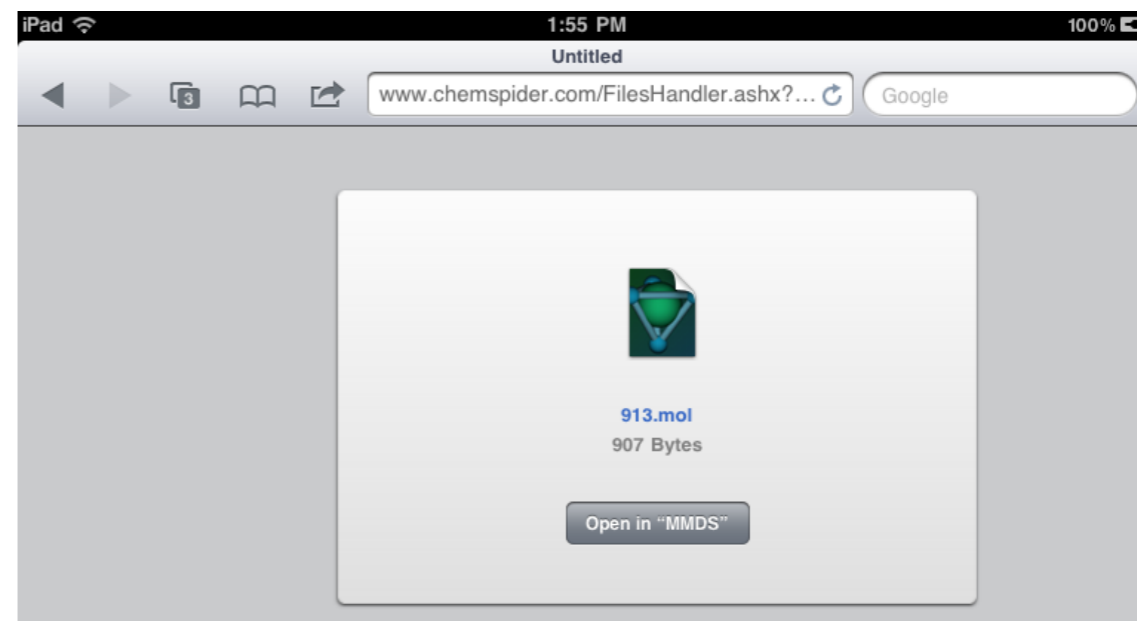
913 (ChemSpider ID)
C₆H₅NO₂

Similar
Wikibox
Mass
PhysChem Properties
Systematic name
pyridine-3-carboxylic acid
SMILES and InChIs
Search Google Scholar

2D 3D Load Save Zoom

Wikipedia Article(s)
Associated Data Sources and Commercial Suppliers
Patents
Articles
Focused Libraries
Names, Synonyms and Database Identifiers
Properties
Medical Subject Headings Classification
Pharmacological Links
SimBioSys LASSO
Spectra
RSC Databases

Contact Feedback Disclaimer Privacy

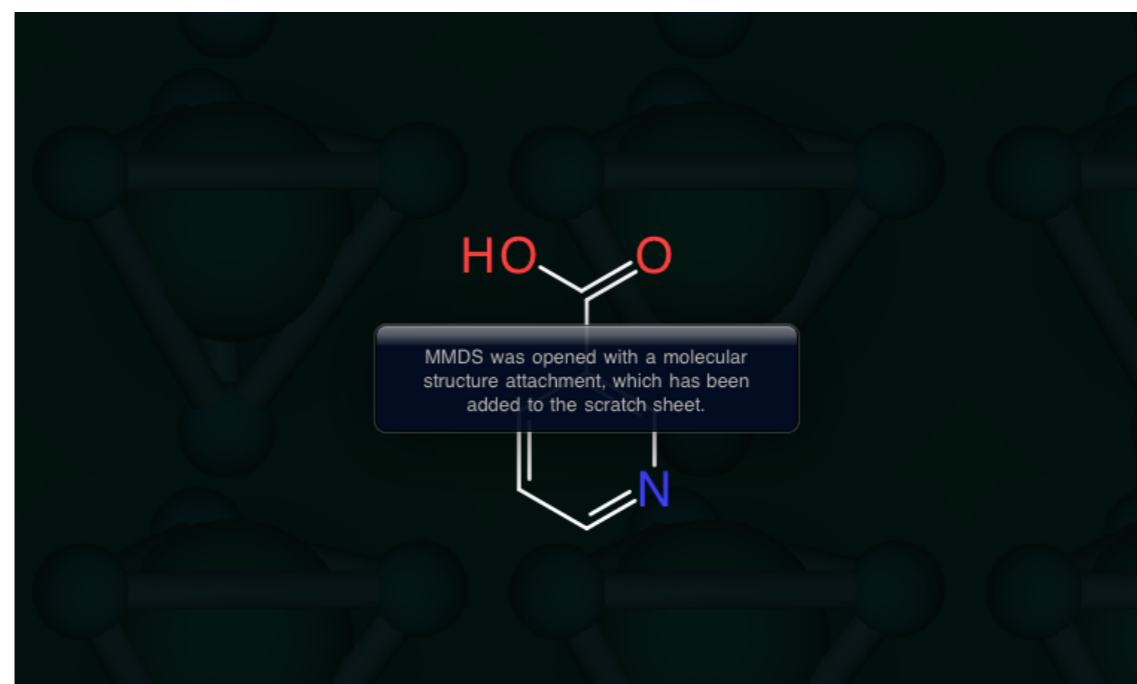


Untitled

www.chemspider.com/FilesHandler.ashx?...

913.mol
907 Bytes

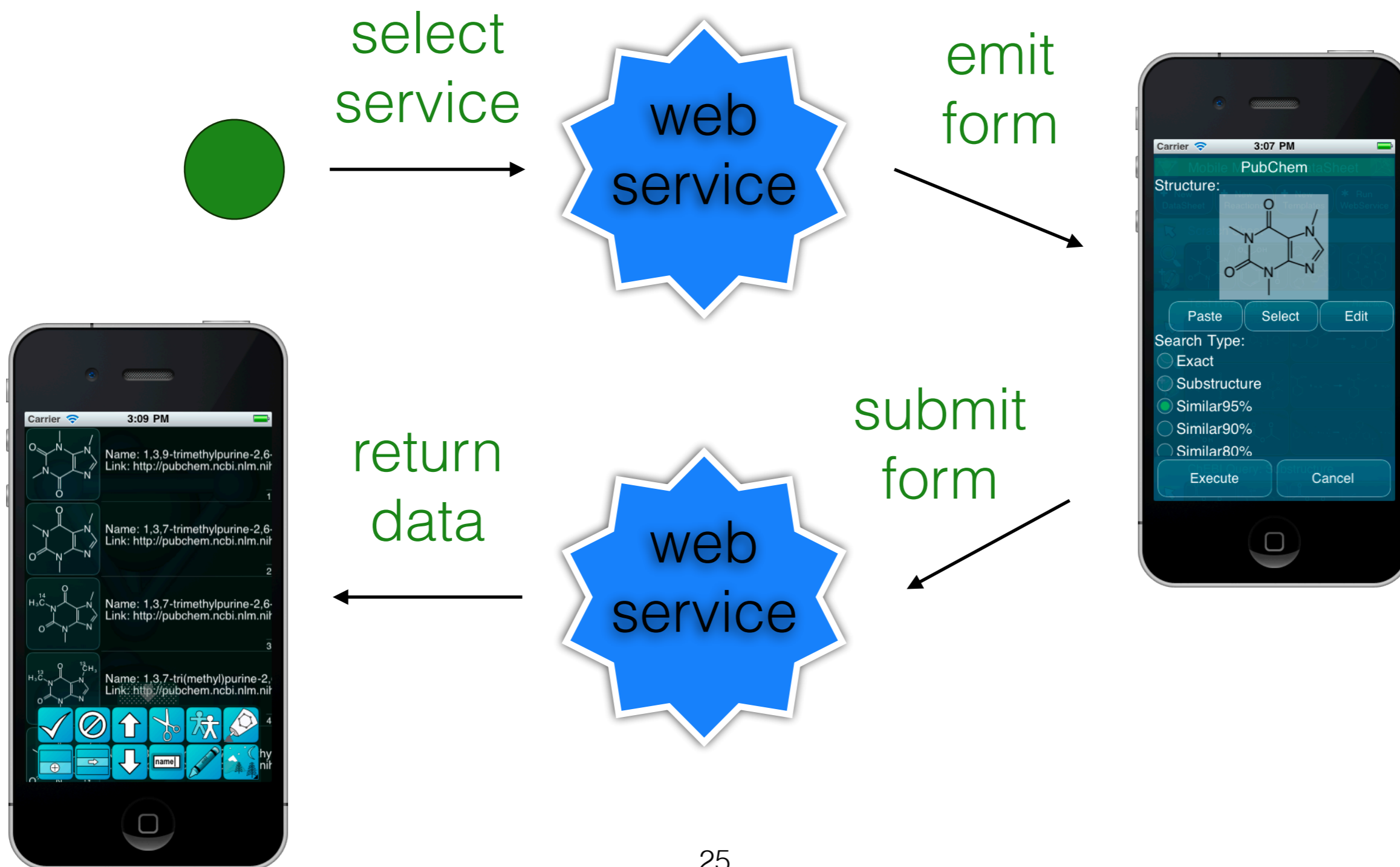
Open in "MMDS"



MMDS was opened with a molecular structure attachment, which has been added to the scratch sheet.

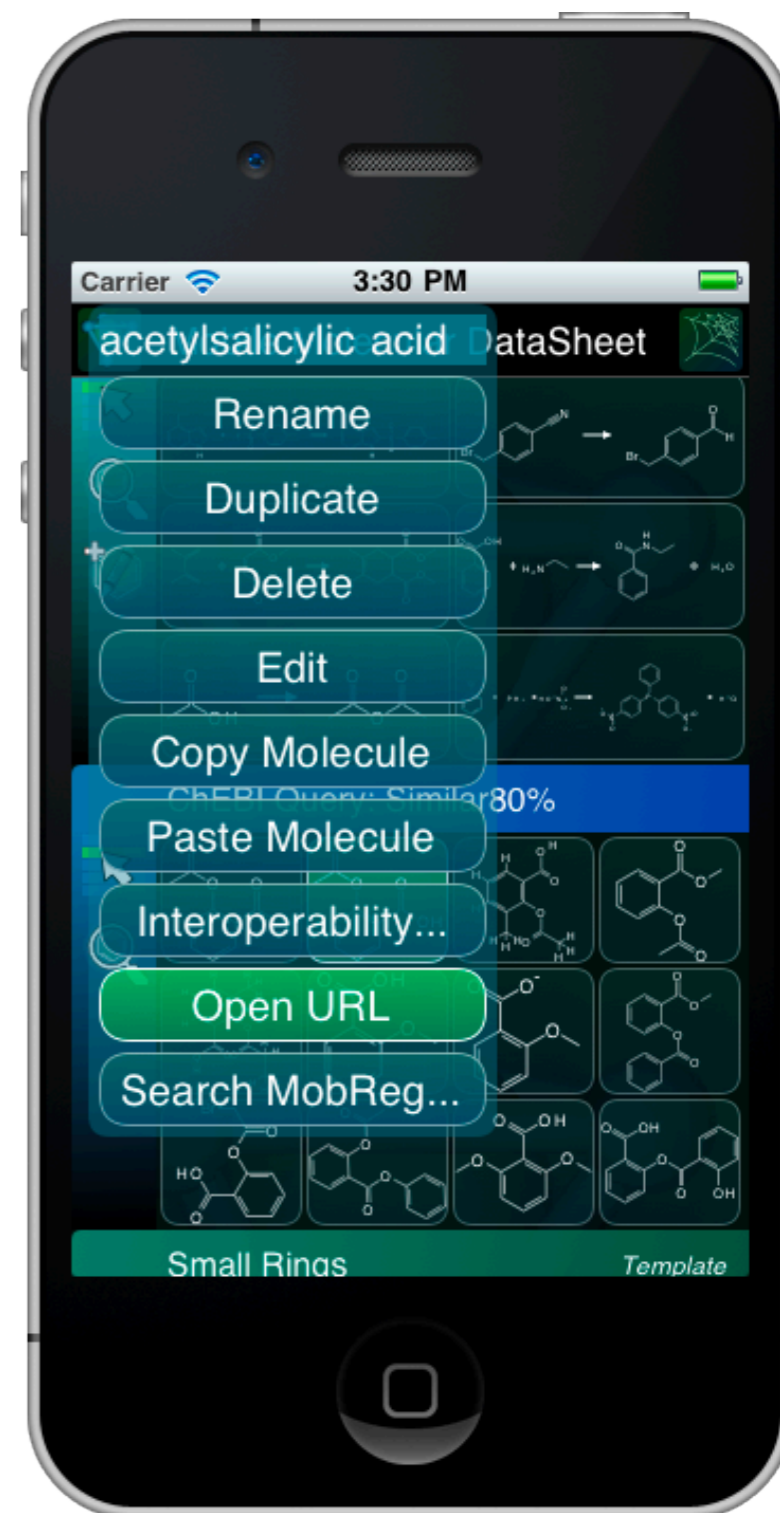
WebServices

- Server protocol defines form-like interface...



Building services

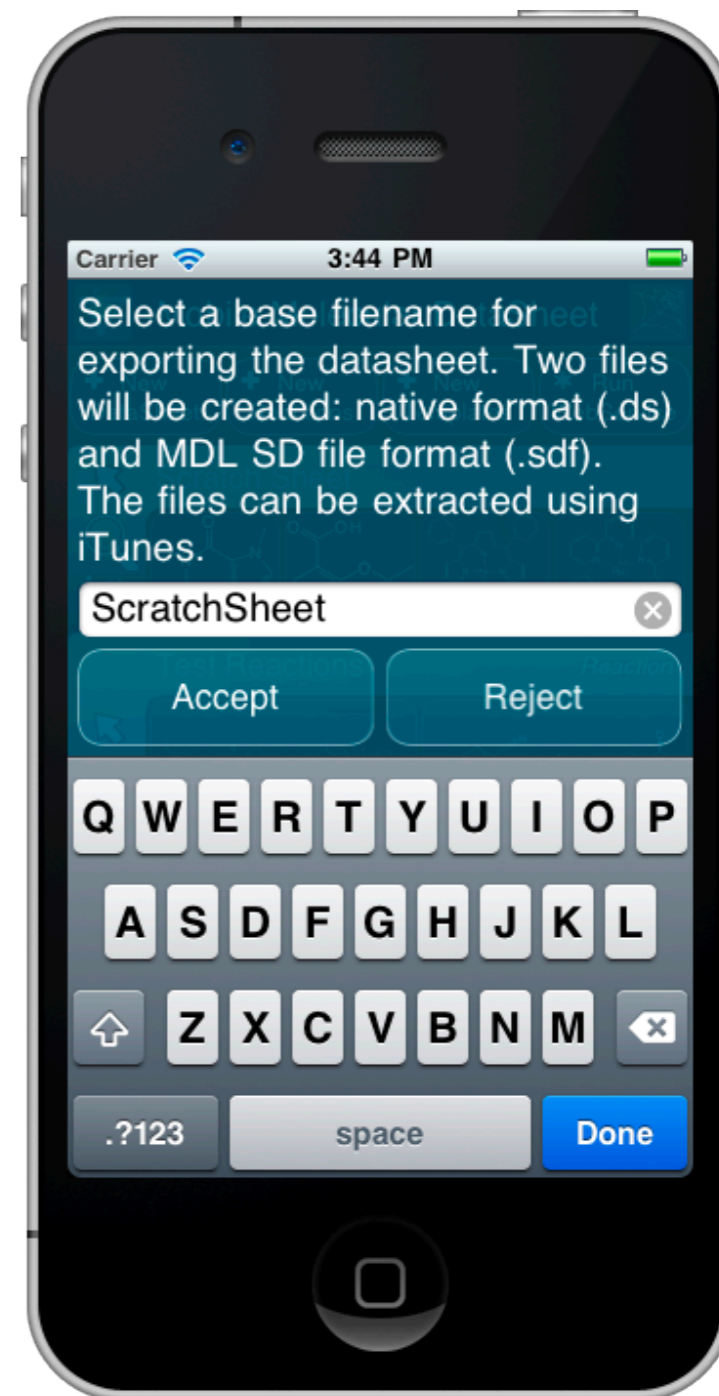
- WebServices use a simple, documented protocol
- Easy to implement custom services with PHP
- **PubChem** and **ChEBI** wrappers available
- Special feature for URL opening...



File transfer

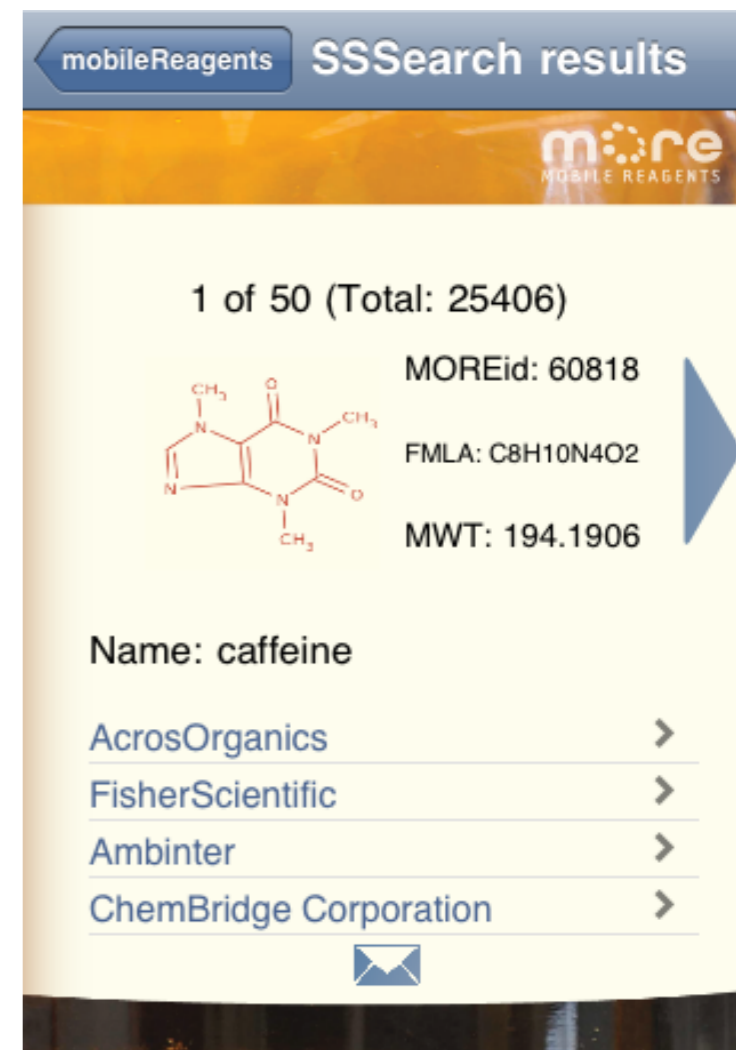
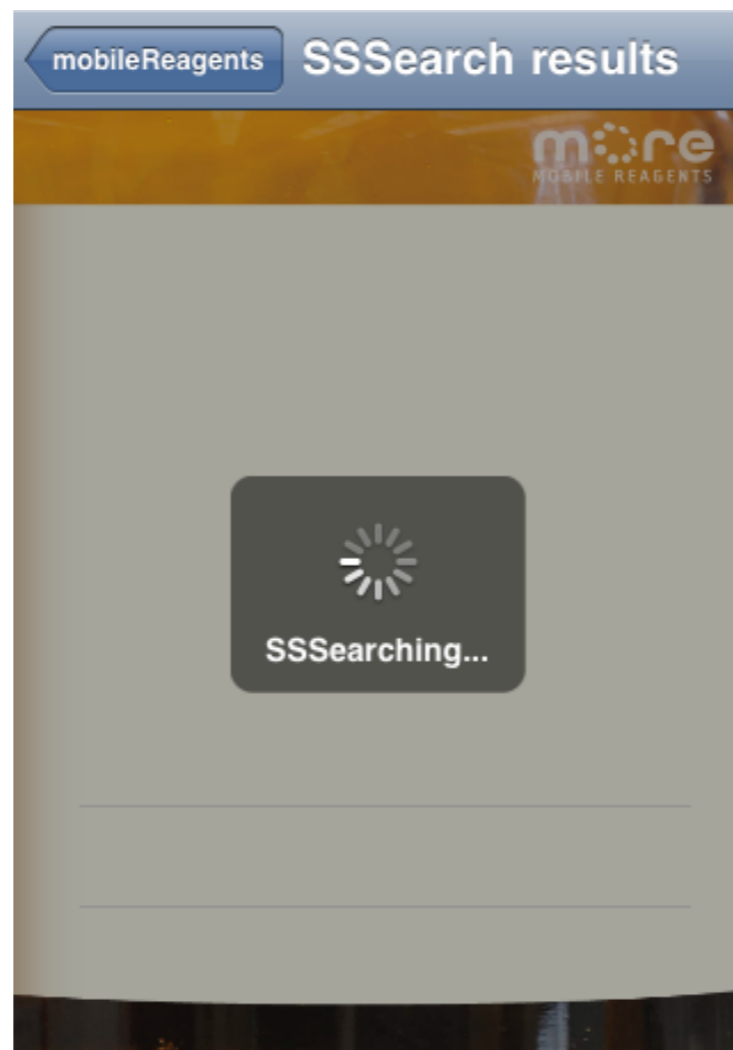


- BlackBerry allows full access to SD card
- iOS allows limited file exchange via iTunes



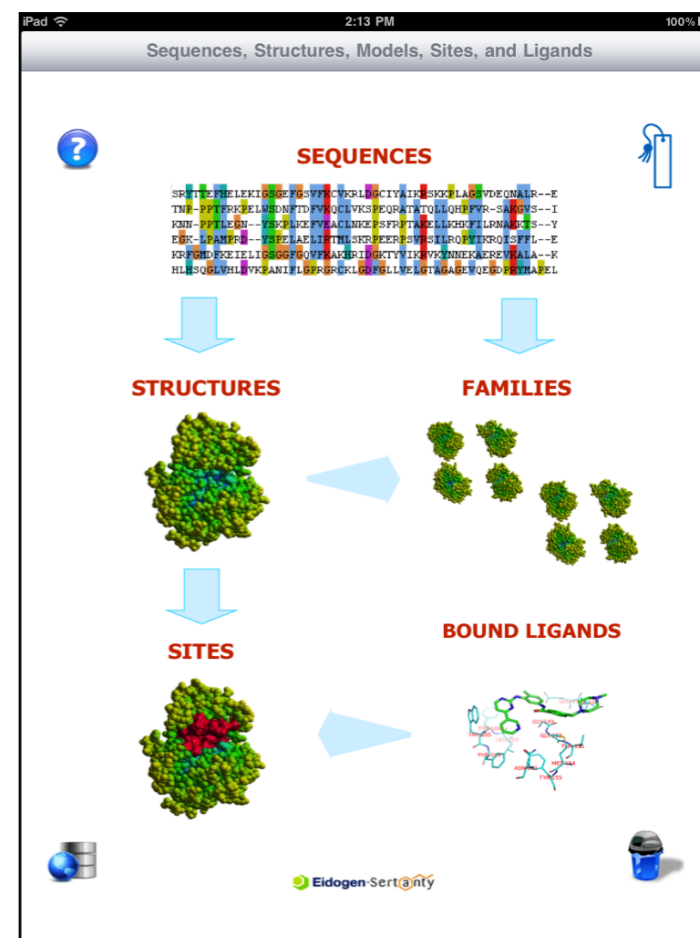
Clipboard and IPC

- Can put chemical data or images onto clipboard, and paste into other apps
- Can also launch other apps...



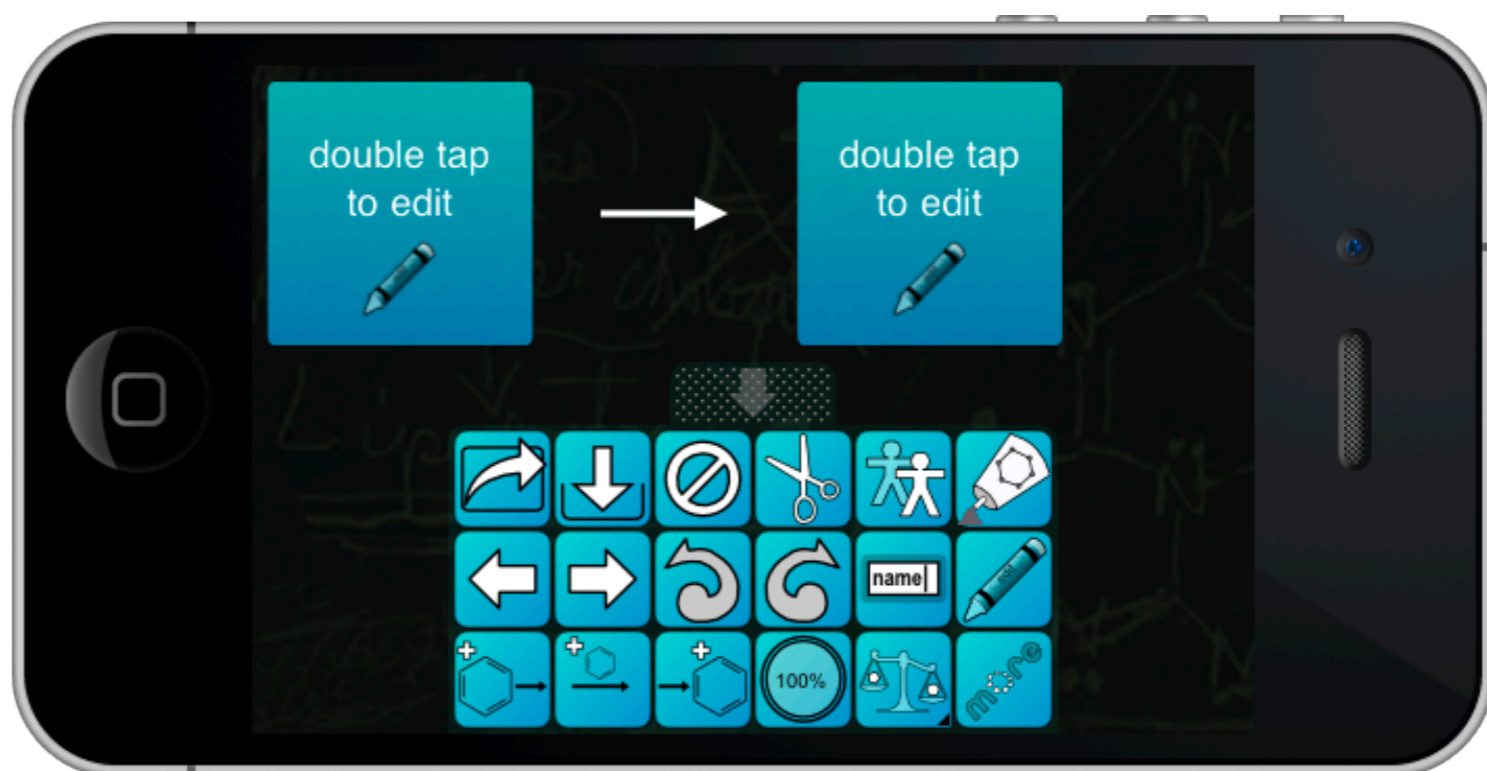
Embedded

- The core tools necessary for a cheminformatics interface have been built...
- ... and are available as a linkable library, for iOS devices.
- **Mobile Reagents** and **iProtein** both use the embedded sketcher.



Reaction101

- Specialised educational app built from MMDS components
- Reaction editing, balancing, Mobile Reagents integration, email, image creation...



Future plans

- The key user-facing cheminformatics components have been built, tested and are commercially available
- Priority now is to integrate these tools into real workflows
- e.g. custom web services, electronic lab notebook client, specialised tools...

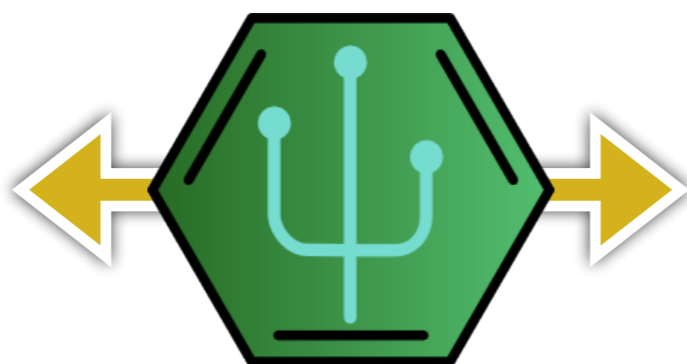
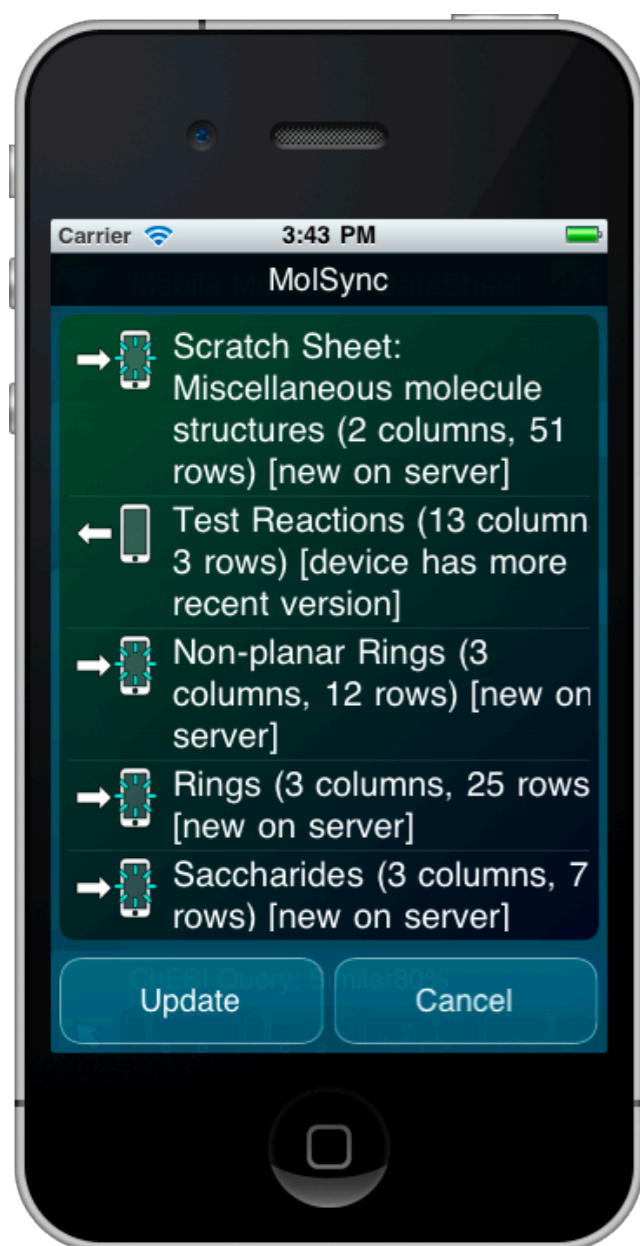
Cloud data

- MMDS makes key **tools** available in a mobile environment...
- ... next step is to make the **data** available.
- Work in progress: [MolSync](#)
- Data synchronisation service



MolSync

- MMDS front end, server API, web interface



The screenshot shows the MolSync web interface in a browser window. The browser address bar displays 'http://domina:8080/MolSync/?panelID=1'. The page header includes the MolSync logo and the text 'Molecular Materials Informatics'. Below the header is an 'Upload' section with a 'Scratch Sheet' table containing 2 columns and 51 rows of chemical structures. Below the Scratch Sheet is a 'Test Reactions' section with 13 columns and 3 rows of chemical reaction schemes. The interface includes navigation buttons like 'More...' and 'Actions'.

Other devices

- iOS, Android, BlackBerry, Windows, Symbian, WebOS, Qt... all incompatible



SYMBIAN

webOS™



- ... only common factor is **HTML5**.

Acknowledgements

<http://molmatinf.com>

- Steve Muskal, Maurizio Bronzetti (Eidogen-Sertanty)
- Greg Landrum, Johannes Maier, Alain Deschenes, Antony Williams, Christoph Steinbeck, Evan Bolton, David Thompson, Rich Apodaca, among others

