Chemistry in Your Pocket

Shrinking cheminformatics applications for mobile devices

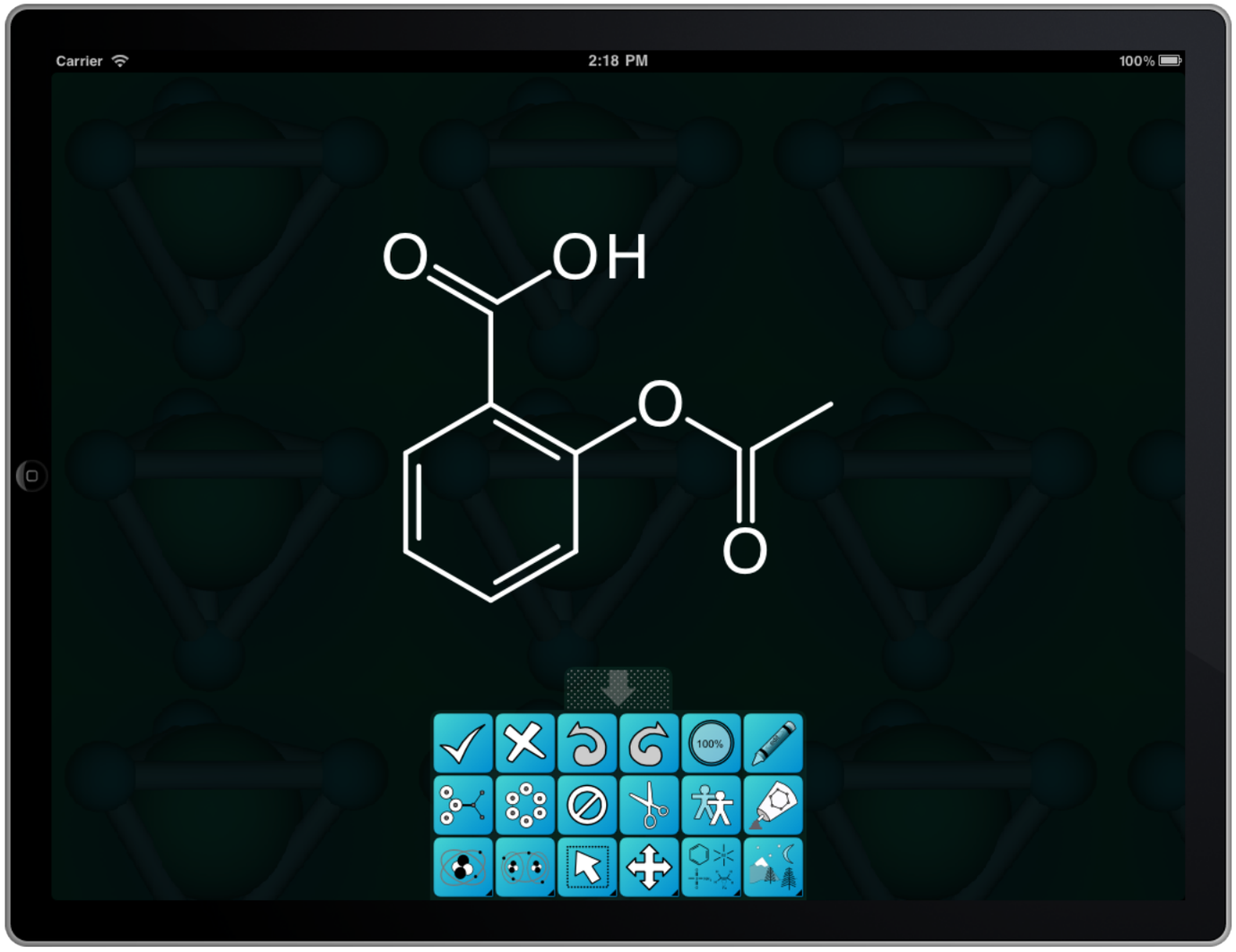
Dr. Alex M. Clark

Anaheim, March 2011

Mobile Molecular DataSheet

Smartphones

Tablets

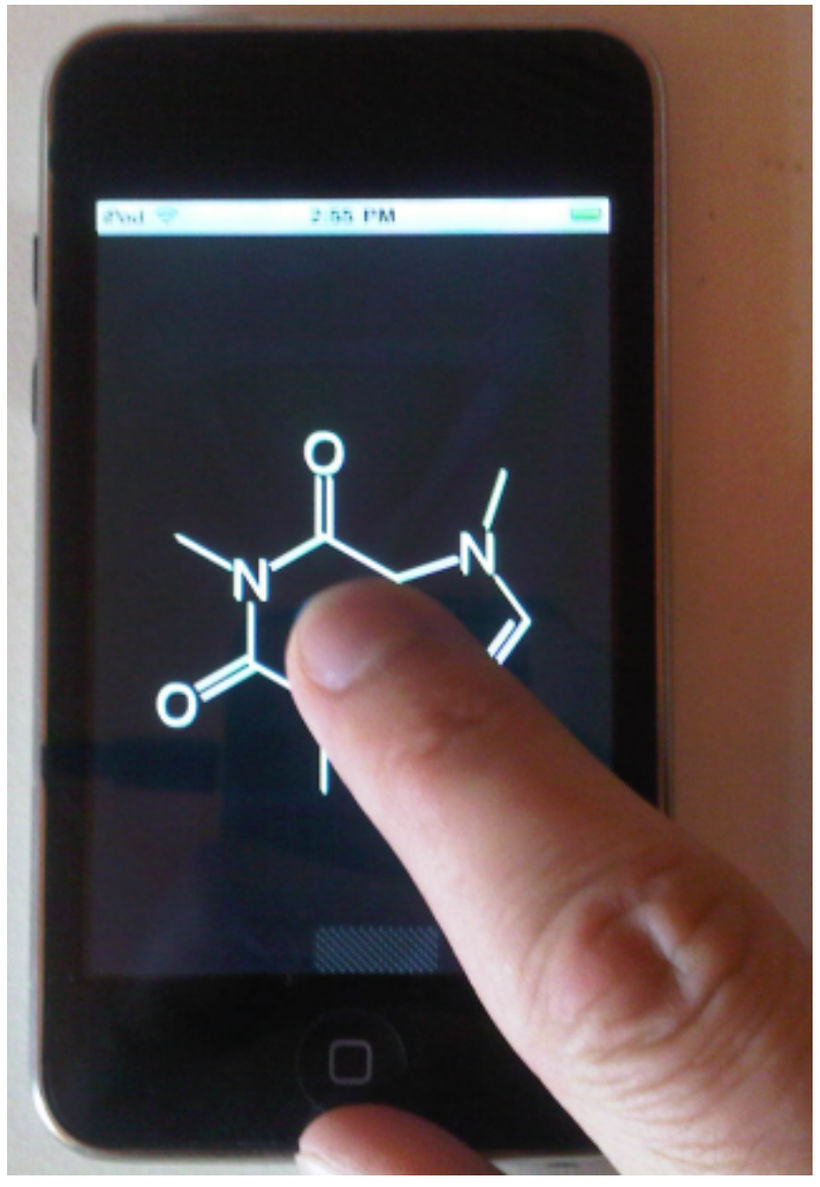


Background

- 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.

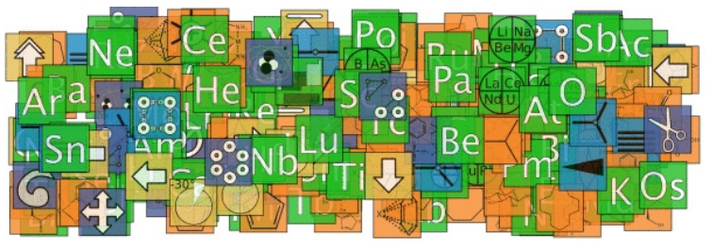
Sketcher challenges

- 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:



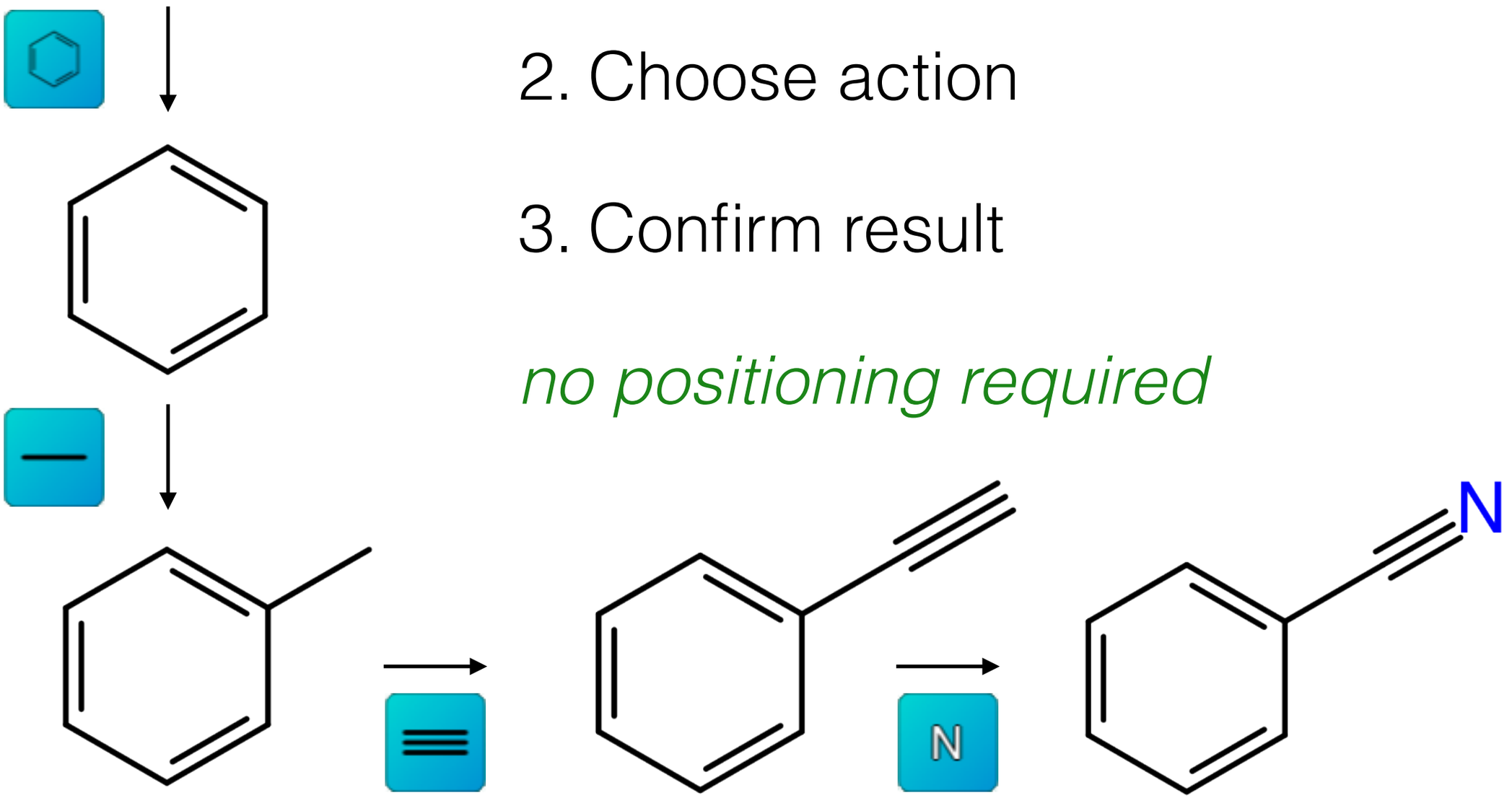
A.M. Clark, **Basic primitives for molecular diagram sketching**, *Journal of Cheminformatics* 2010, **2**:8.

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

Sketching primitives

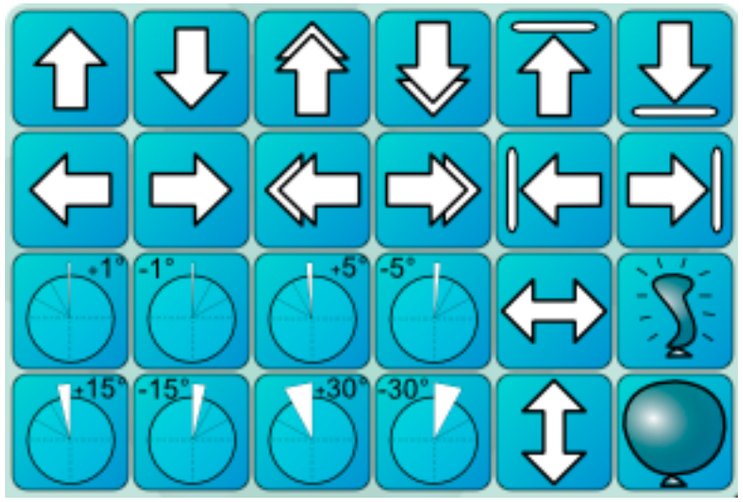
1. Pick atoms/bond
2. Choose action
3. Confirm result

no positioning required



Primitives


100%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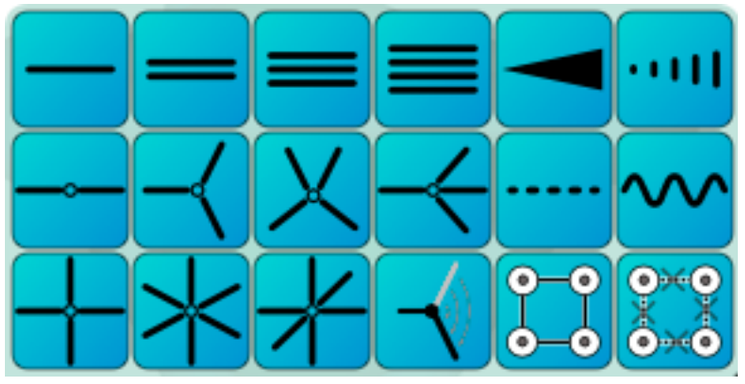

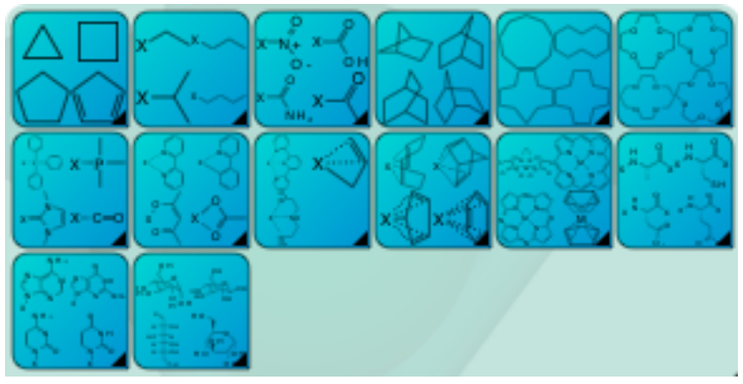

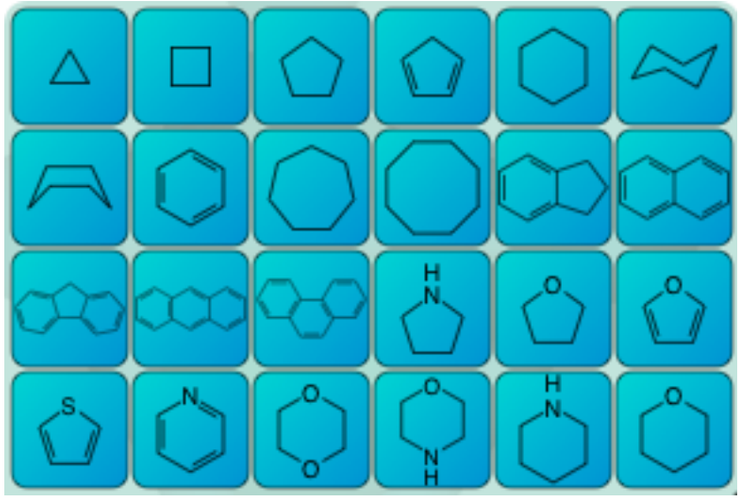


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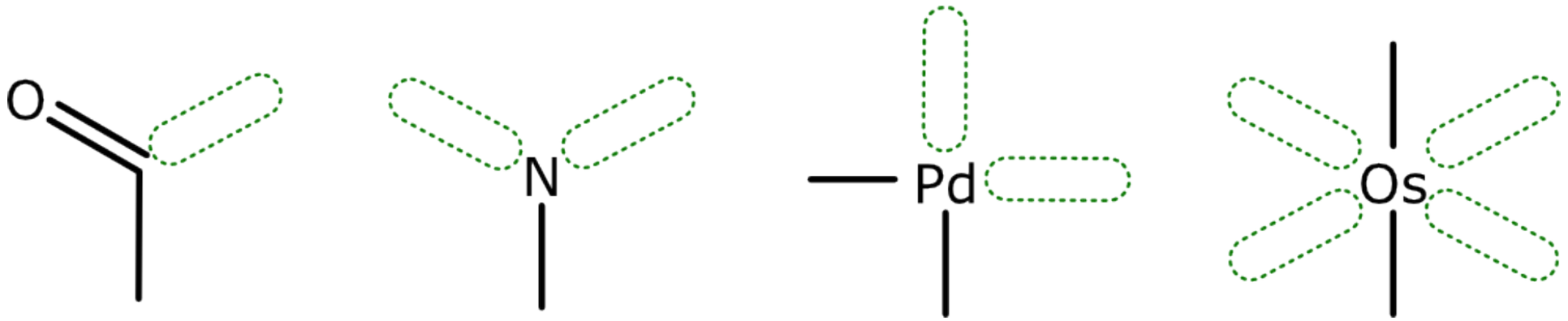
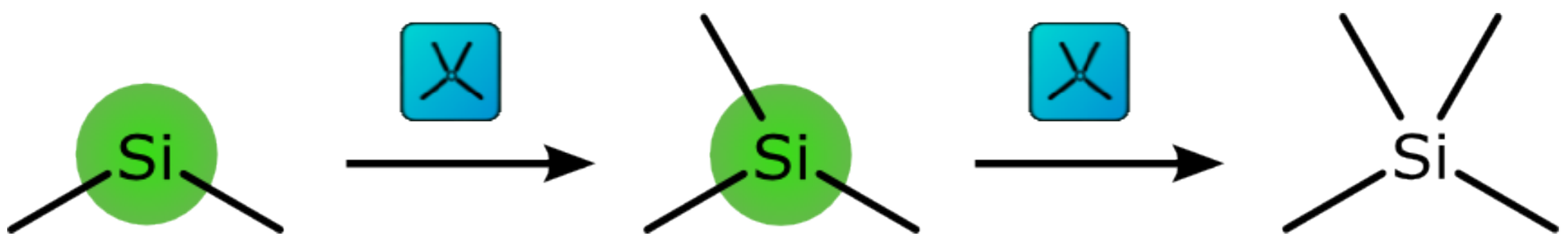
Geometry

- Convenient sketching by guestimating geometry



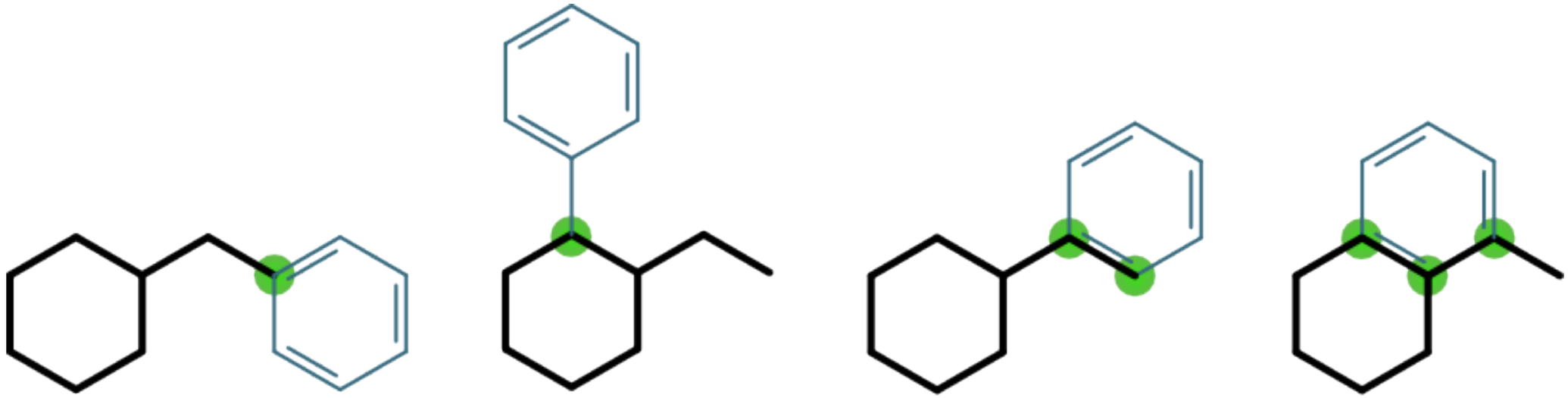
- Or specifying explicitly



Templates

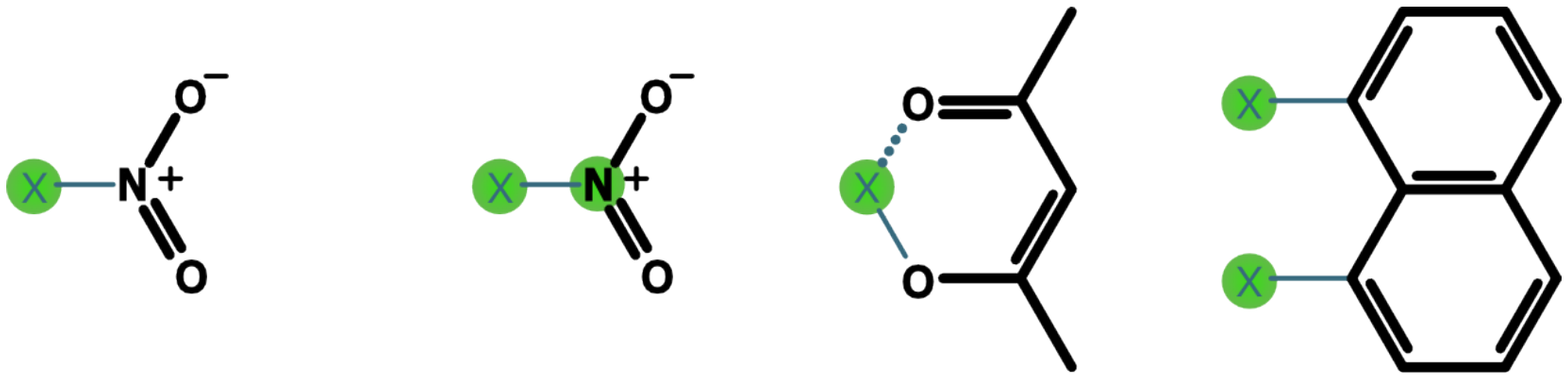
- Multiple fusion modes, multiple results

unguided



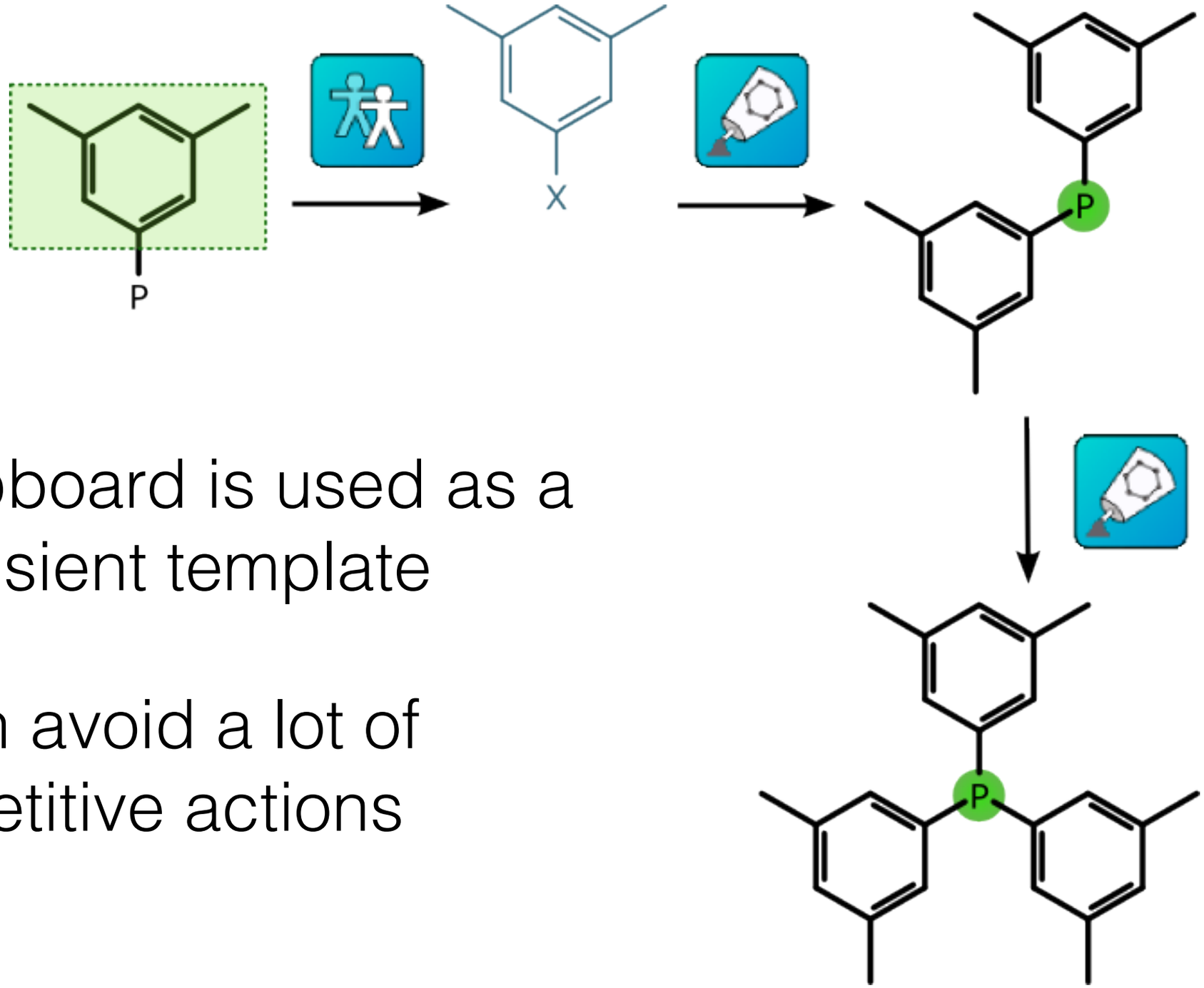
atom bridge bond multi

guided



atom bond chelate multi

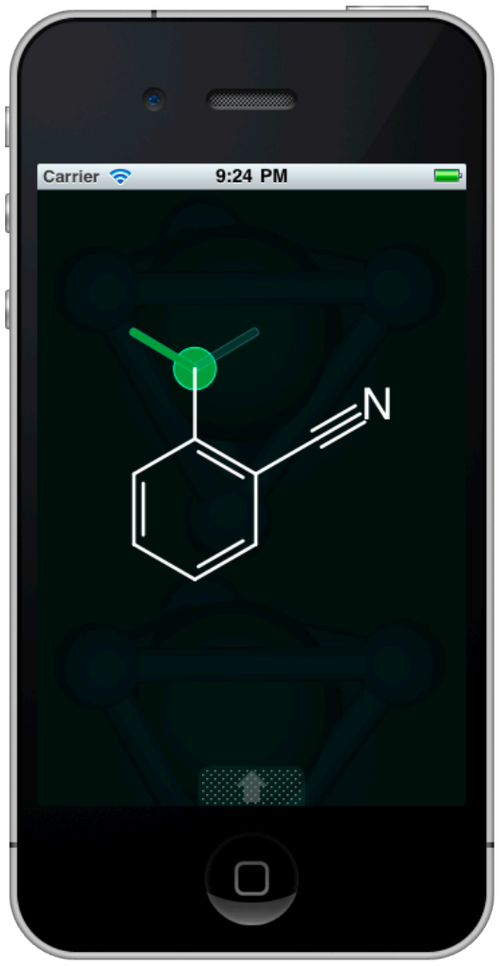
Clipboard



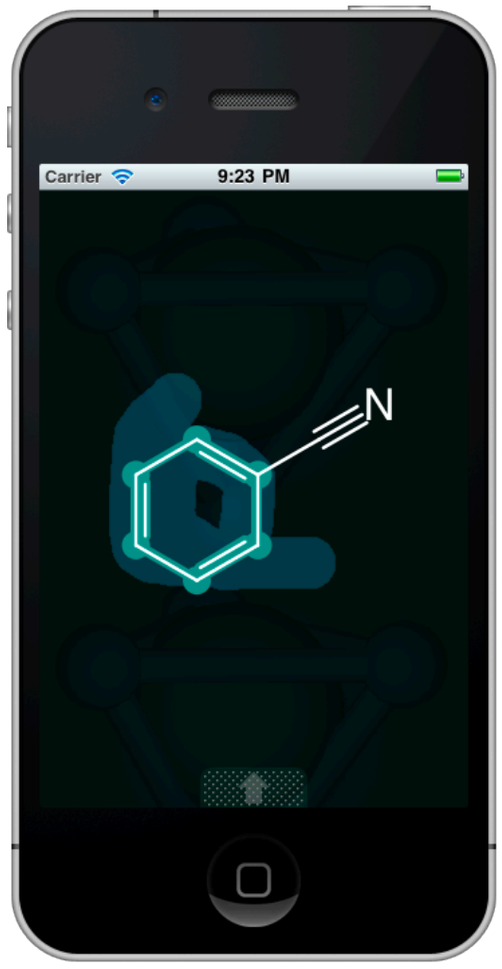
- Clipboard is used as a transient template
- Can avoid a lot of repetitive actions

Gestures

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



Finger drawing

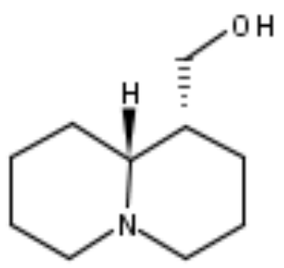
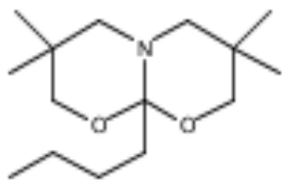


Crayon selection

Context menus

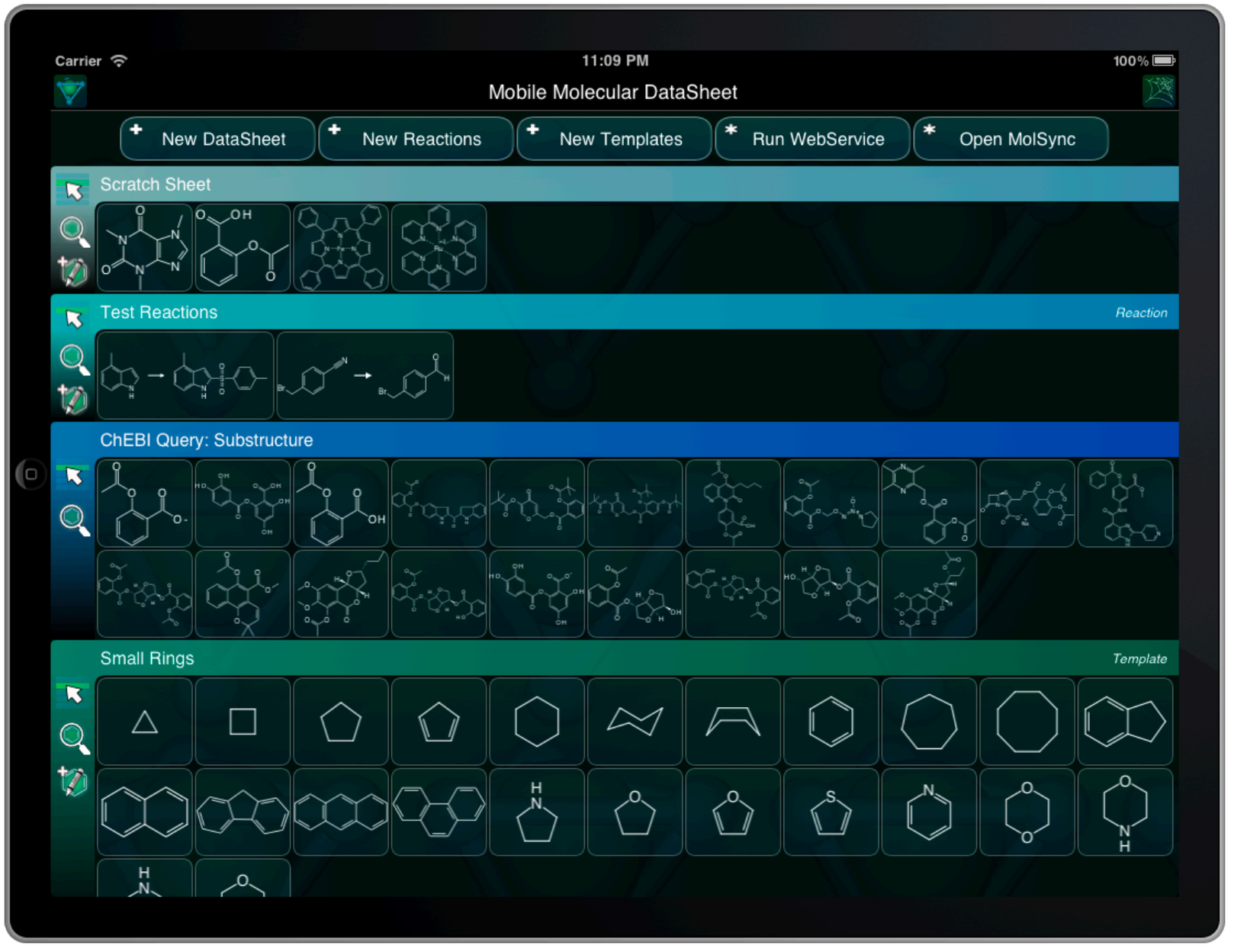
Now what?

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

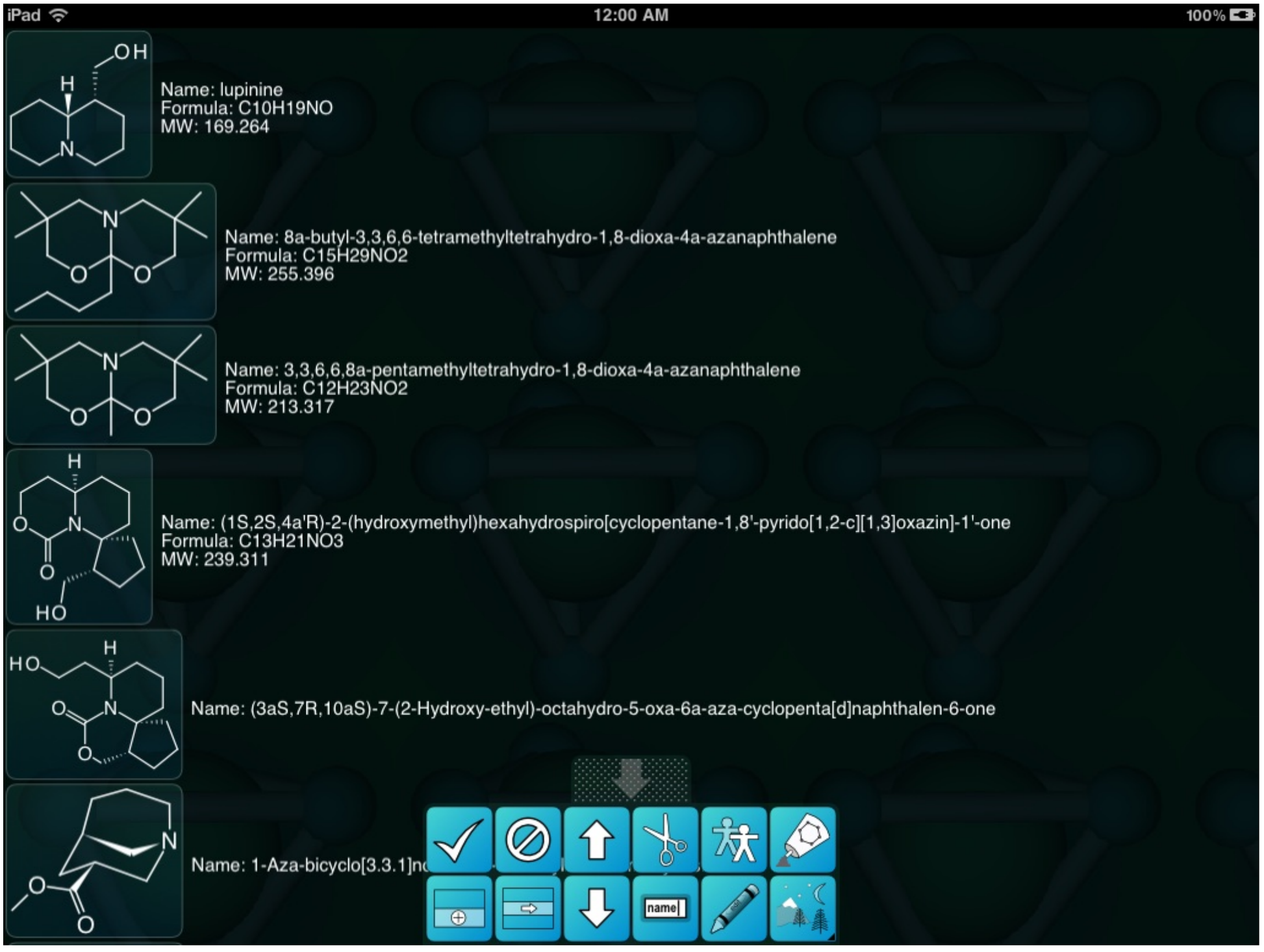
	Molecule	Name	Formula	MW
1		lupinine	C10H19NO	169.264
2		8a-butyl-3,3,6,6-tetramethyltetra	C15H29NO2	255.3963
3		3,3,6,6,8a-pentamethyltetrahydr	C12H23NO2	213.31656

Directory of DataSheets

- Represent each row with a molecule glyph:



Detail view

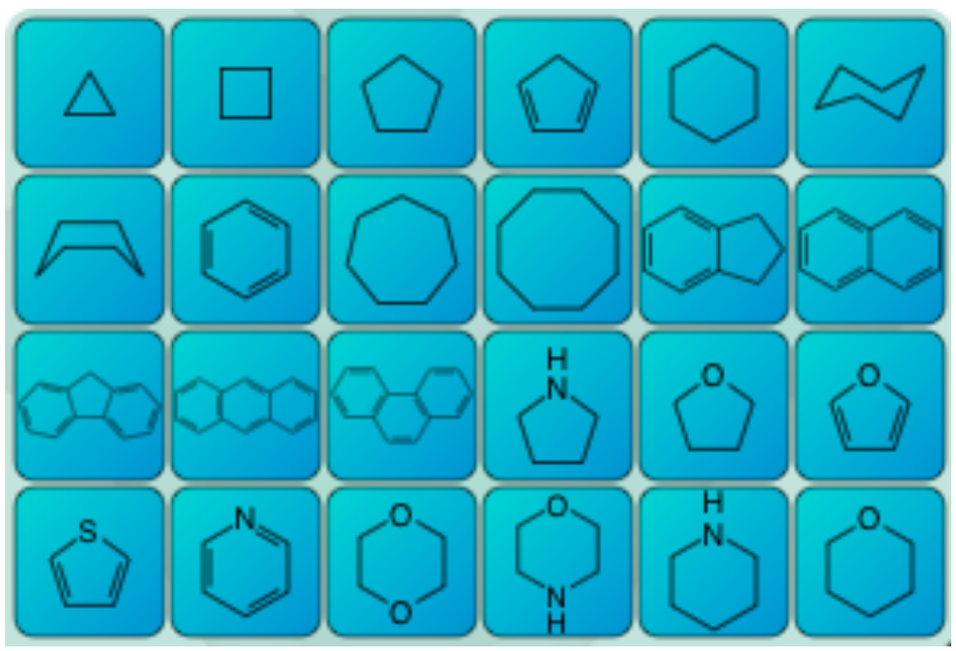

iPad
12:00 AM
100%
Name: lupinine
Formula: C10H19NO
MW: 169.264
Name: 8a-butyl-3,3,6,6-tetramethyltetrahydro-1,8-dioxa-4a-azanaphthalene
Formula: C15H29NO2
MW: 255.396
Name: 3,3,6,6,8a-pentamethyltetrahydro-1,8-dioxa-4a-azanaphthalene
Formula: C12H23NO2
MW: 213.317
Name: (1S,2S,4a'R)-2-(hydroxymethyl)hexahydrospiro[cyclopentane-1,8'-pyrido[1,2-c][1,3]oxazin]-1'-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]n
name

Editing

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

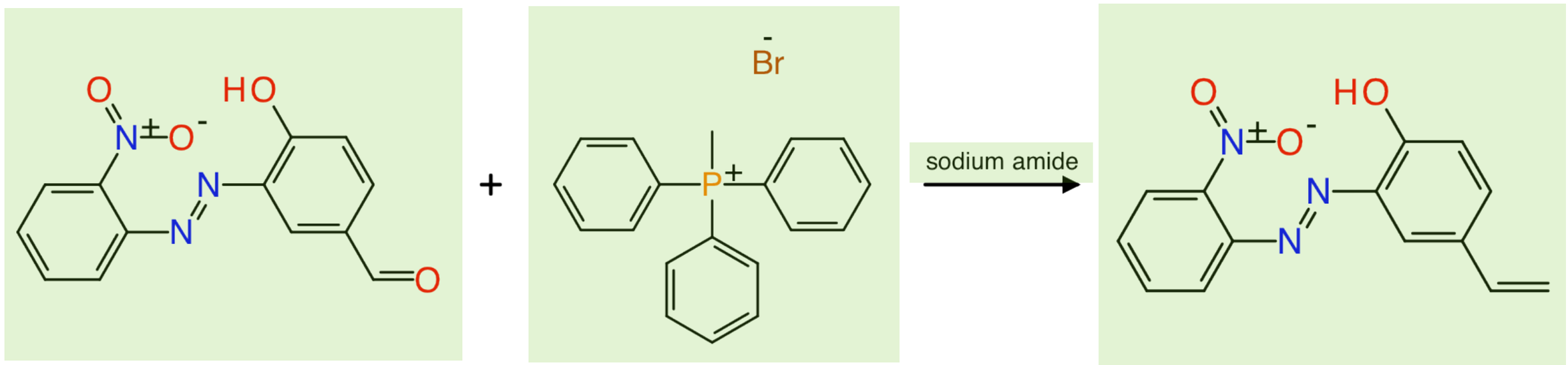
Templates

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



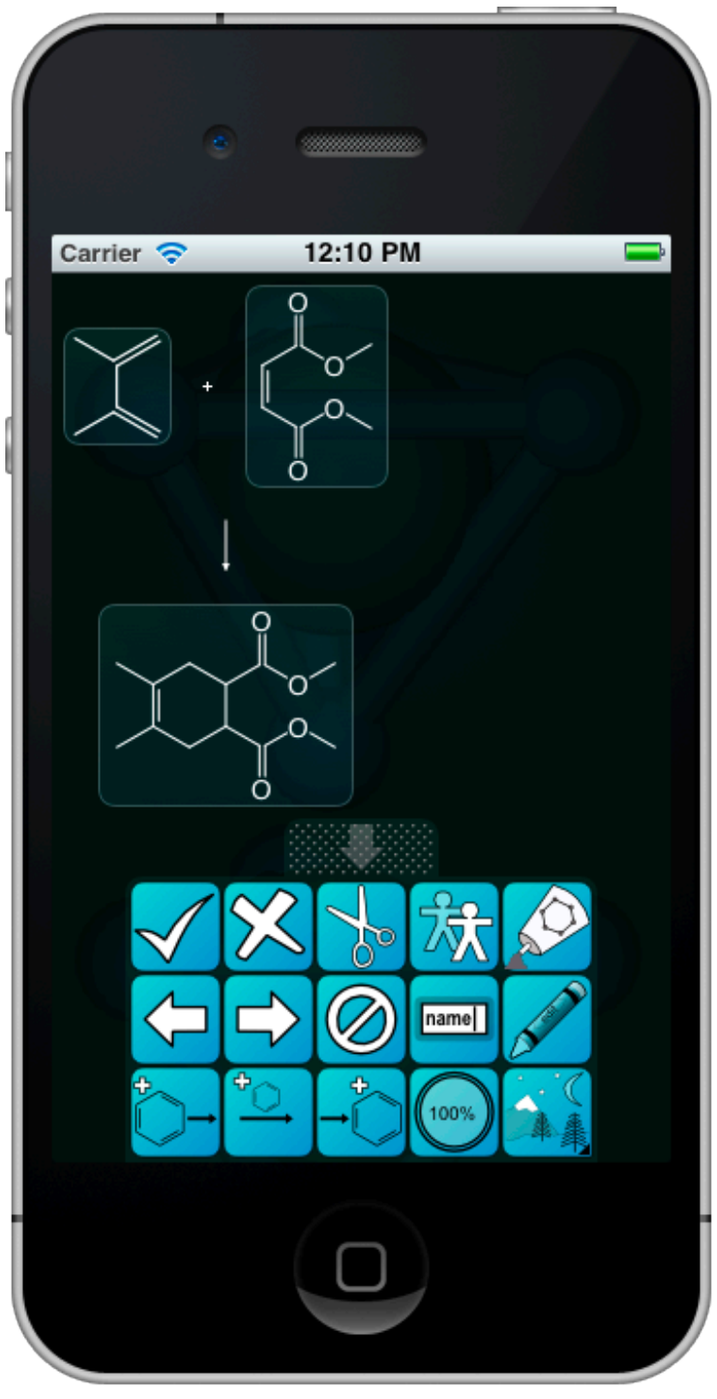
Reactions

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

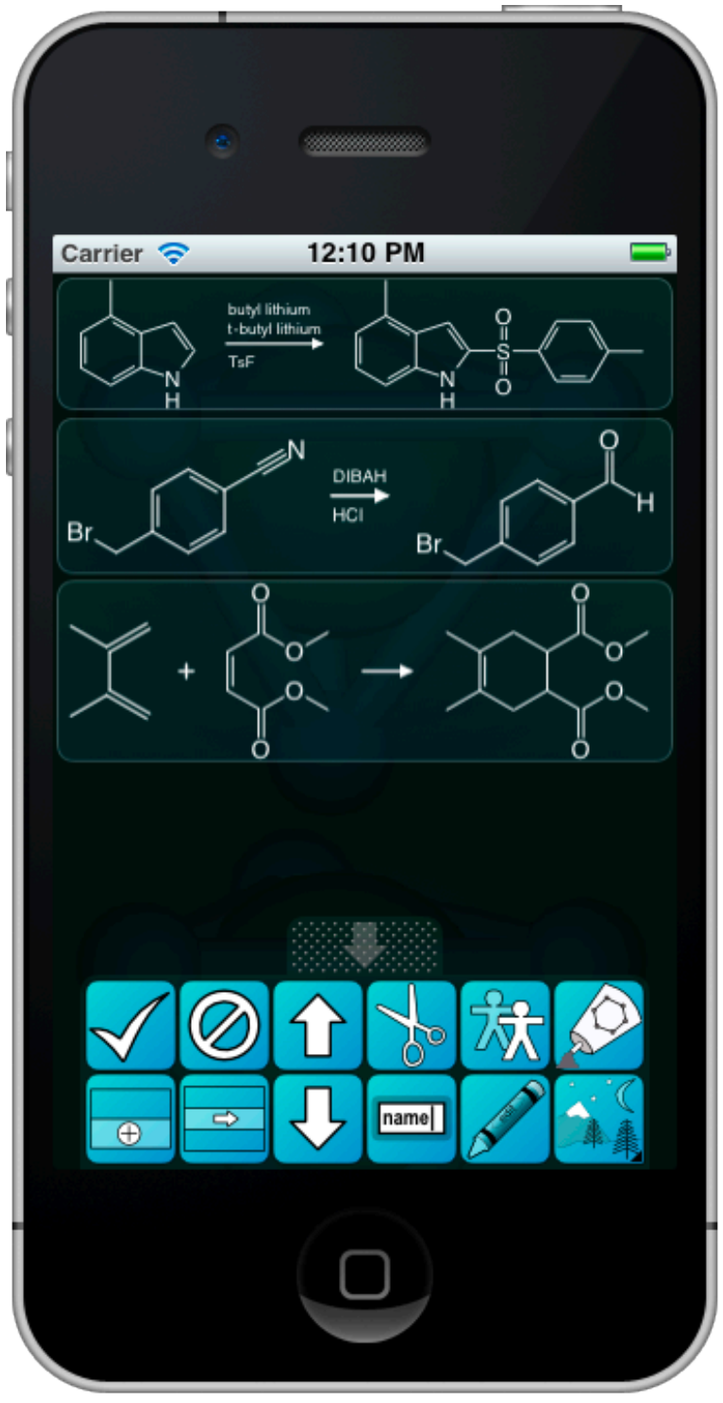


A **B** **C** **D**

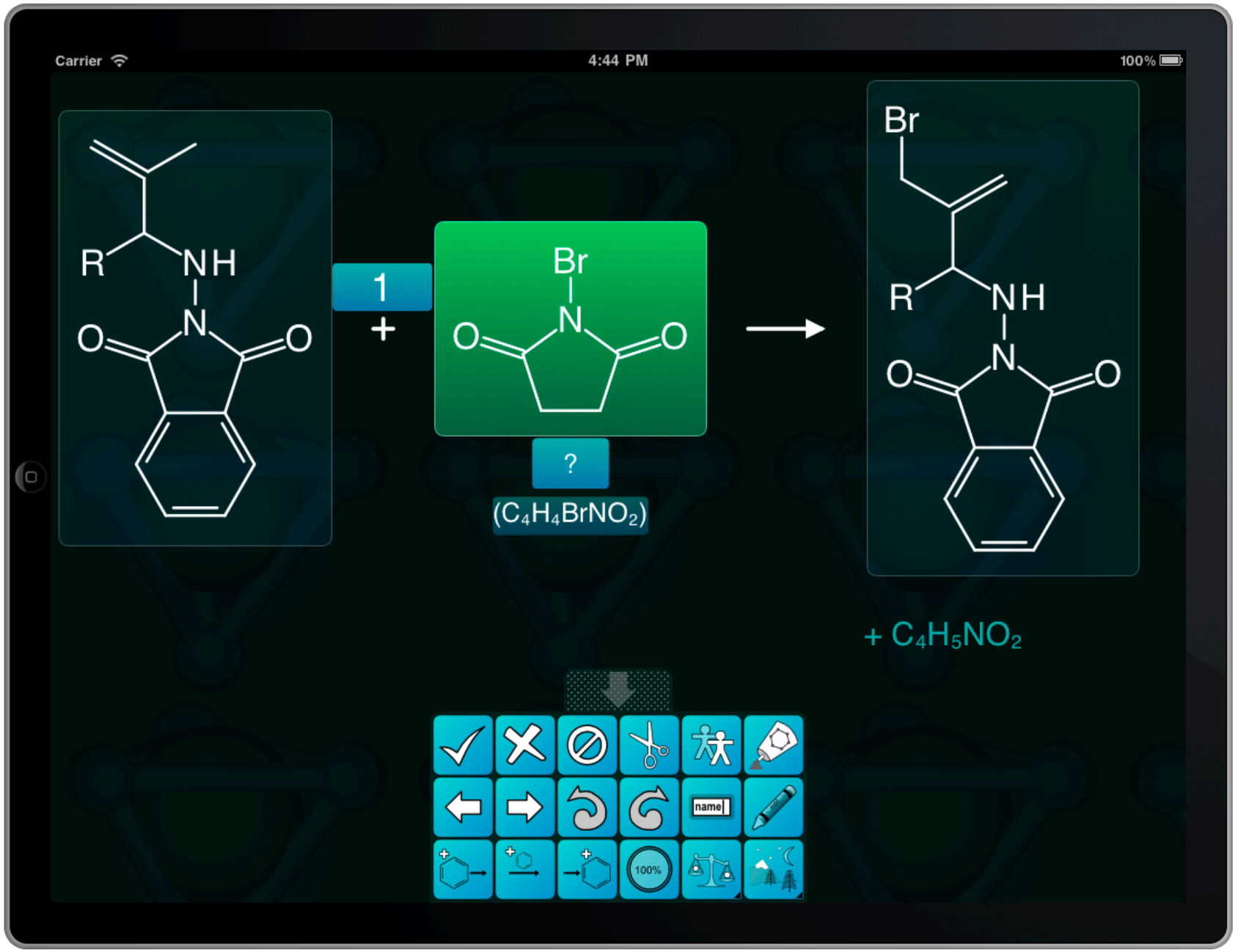
Reaction editing



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

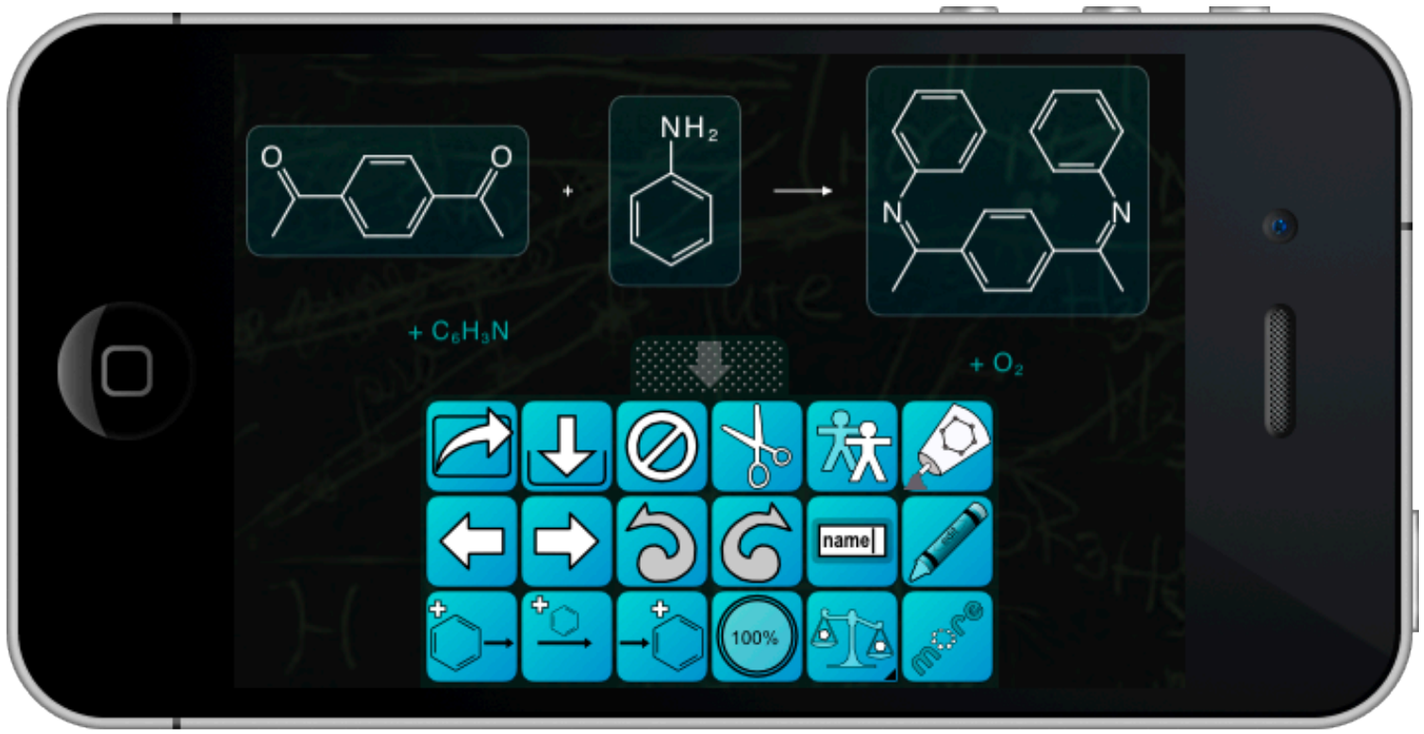


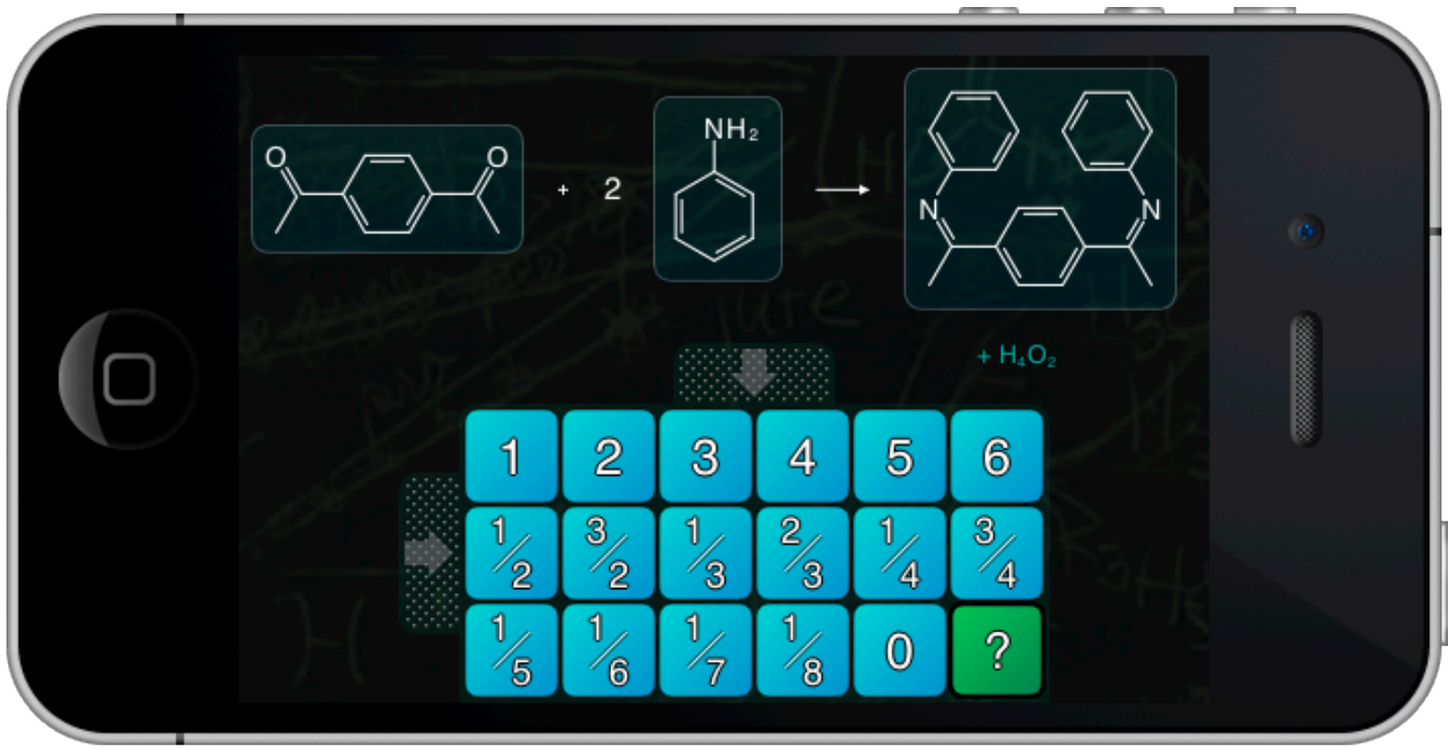
On tablets



- Landscape on iPad is ideal

Stoichiometry



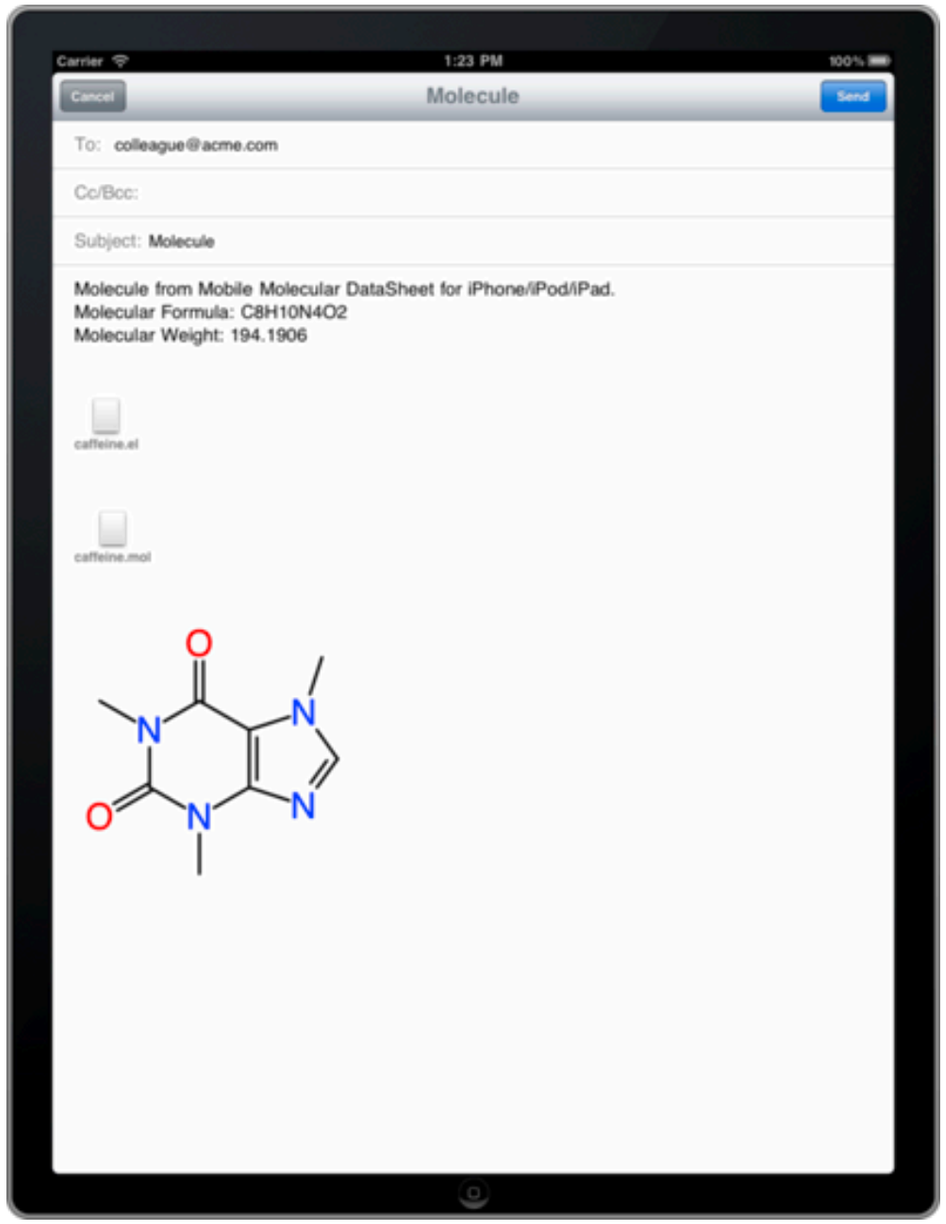


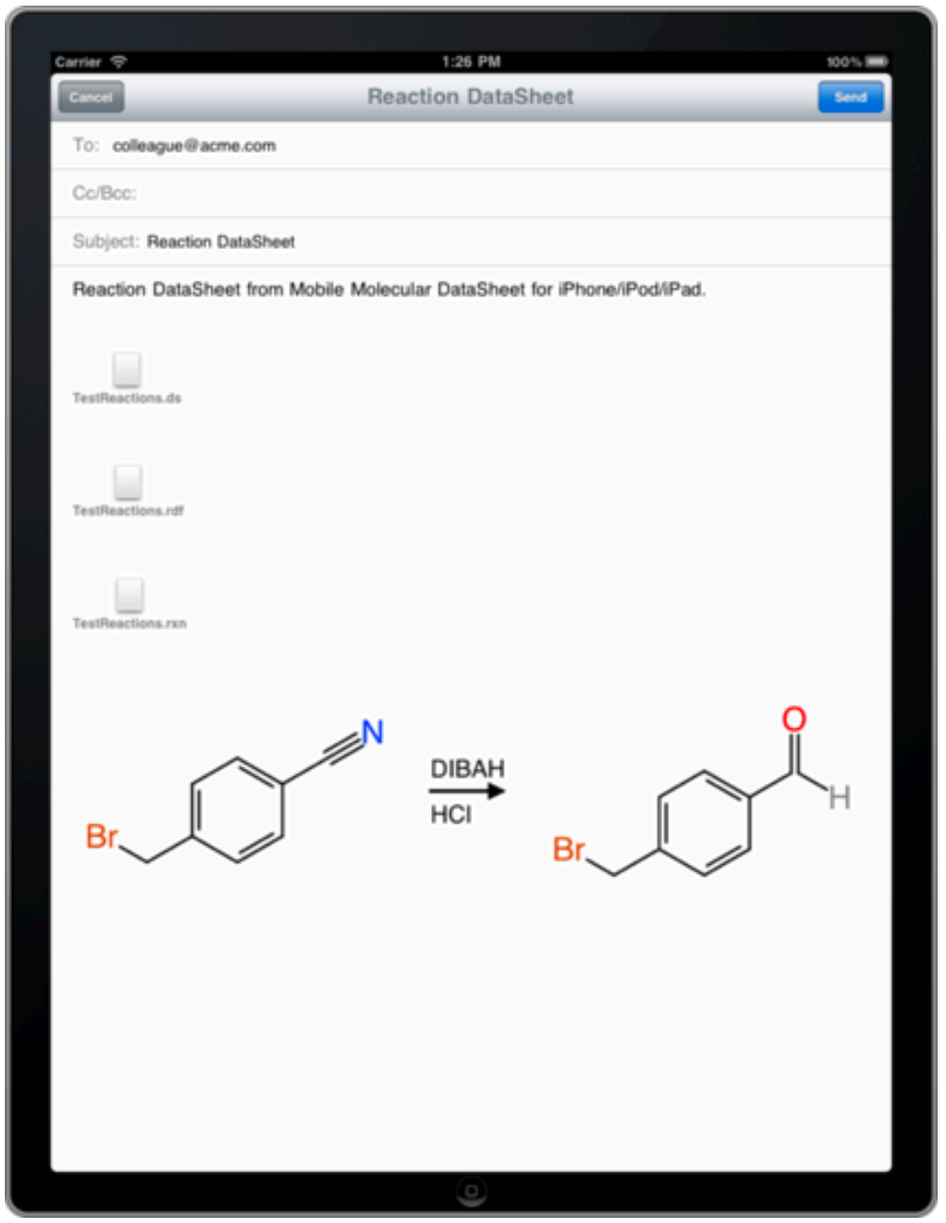
Communication

- 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:



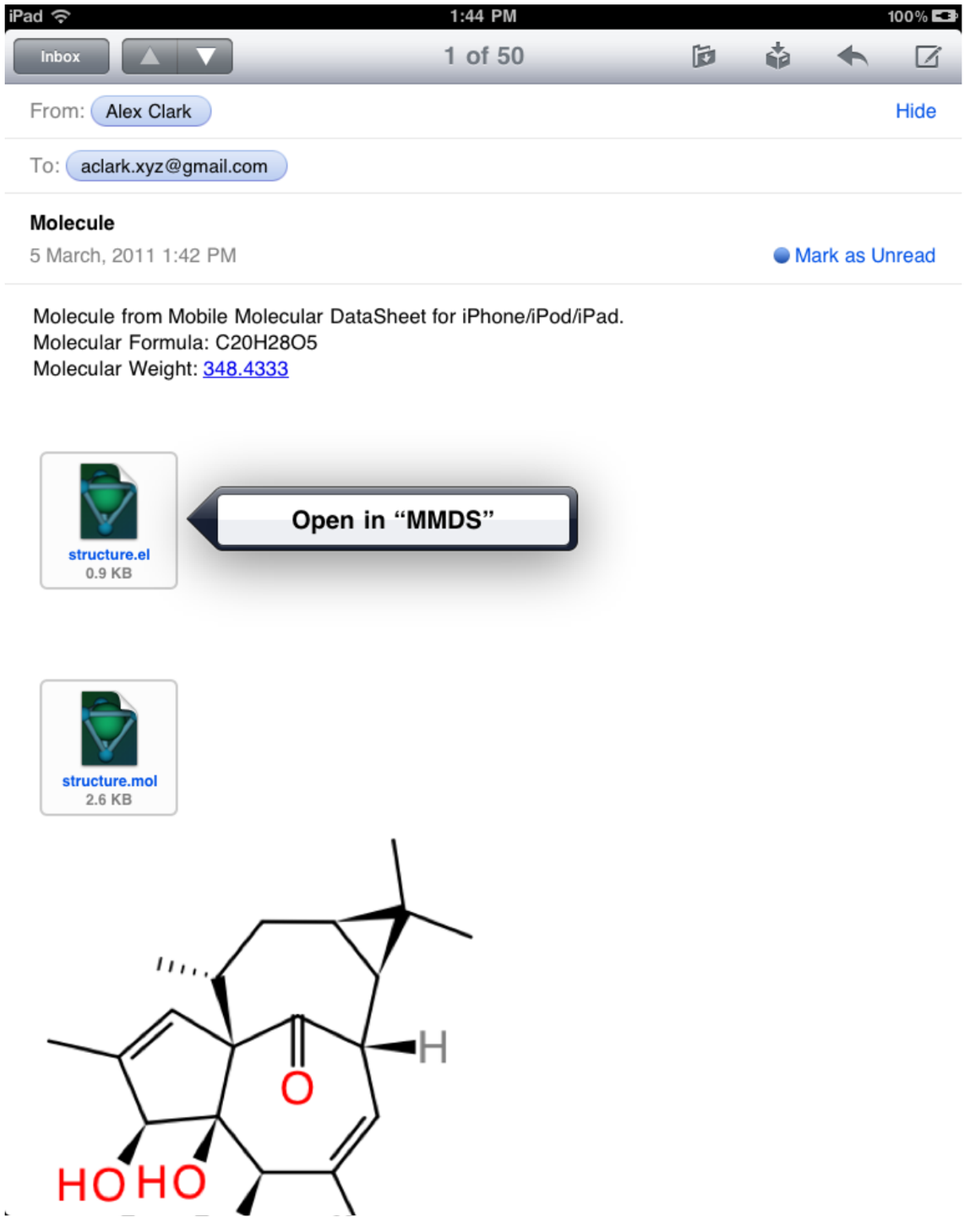


Receiving email

- Attachments include industry standard formats (MDL), file extensions and MIME types

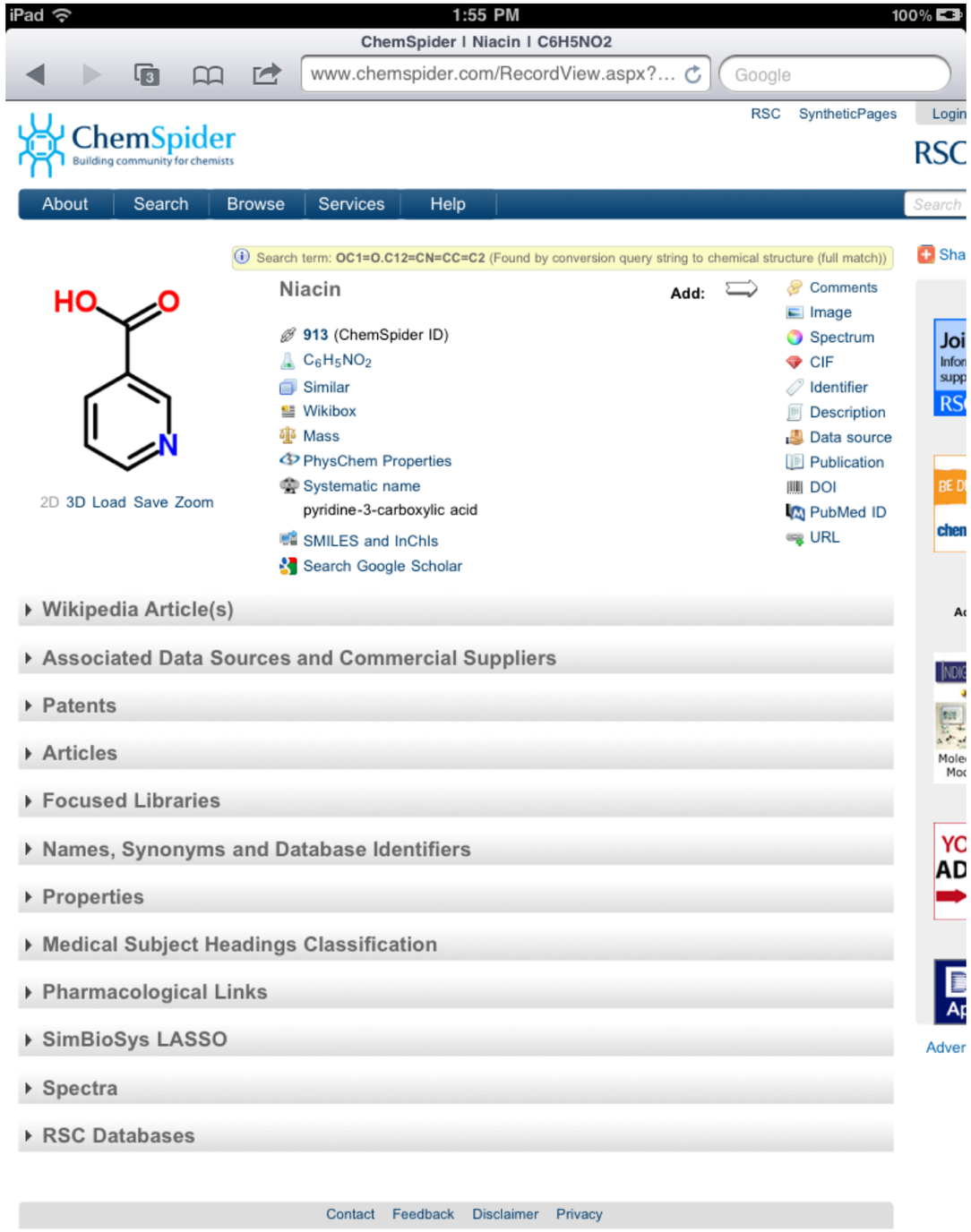
- Exchange data with other mobile users, or the outside world

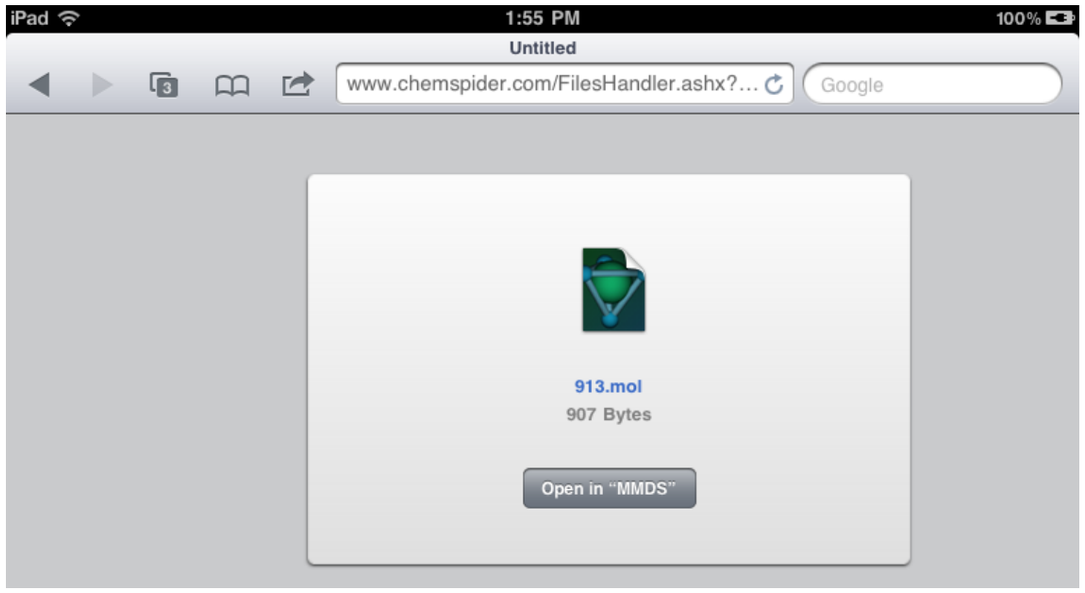
- Opens directly into app...

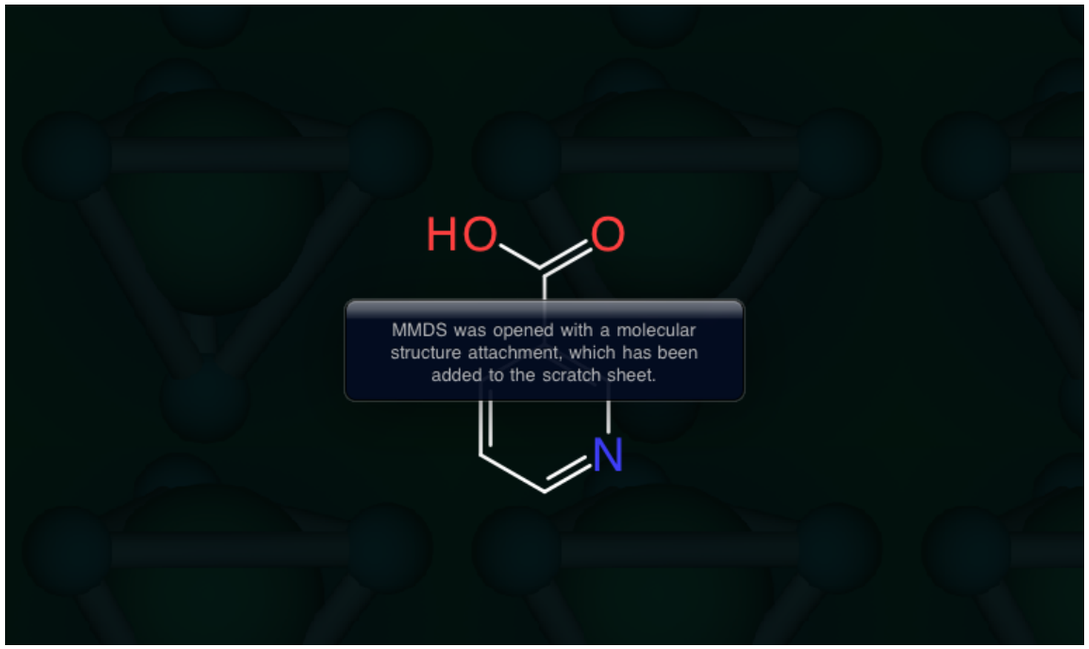


Web downloads

- Same mechanism as attachments...

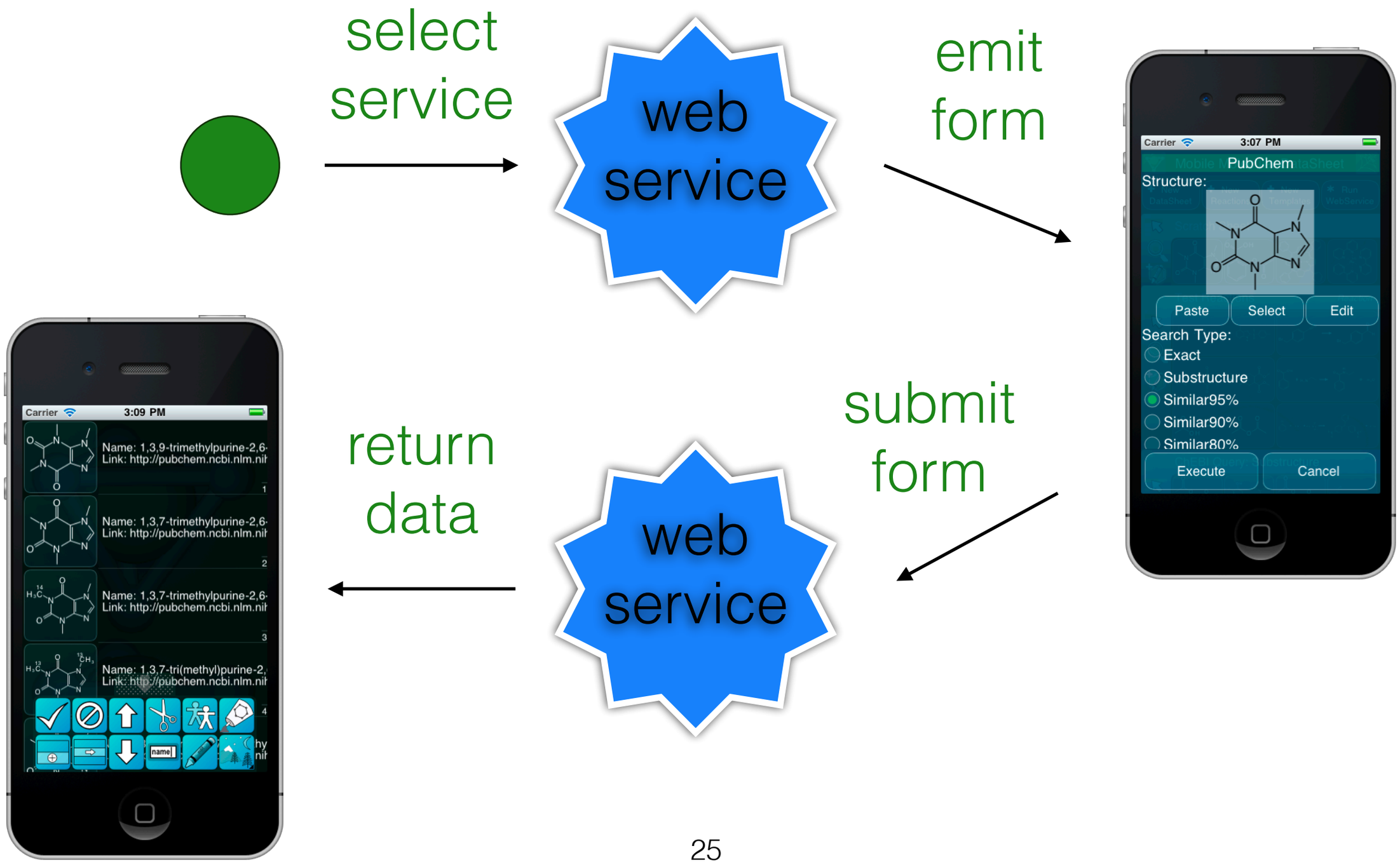






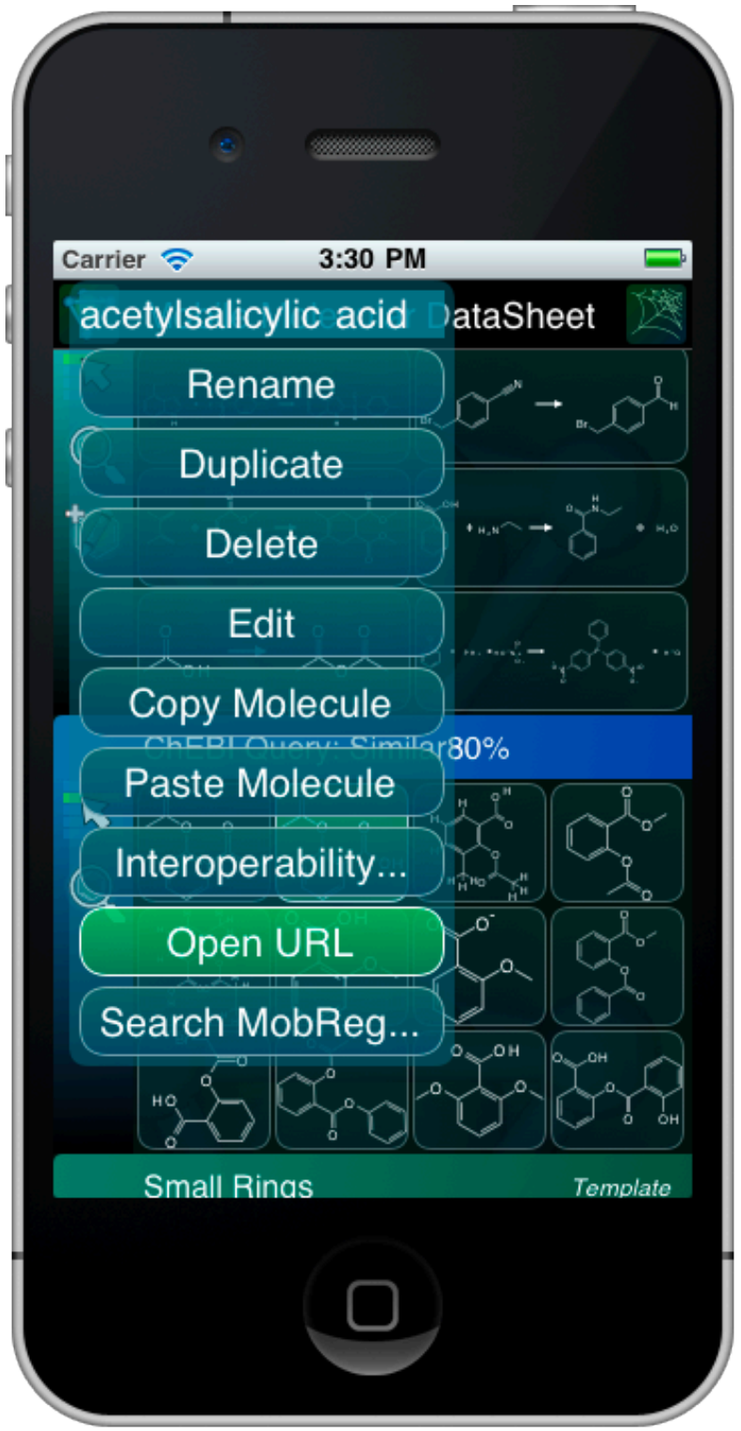
WebServices

- Server protocol defines form-like interface...



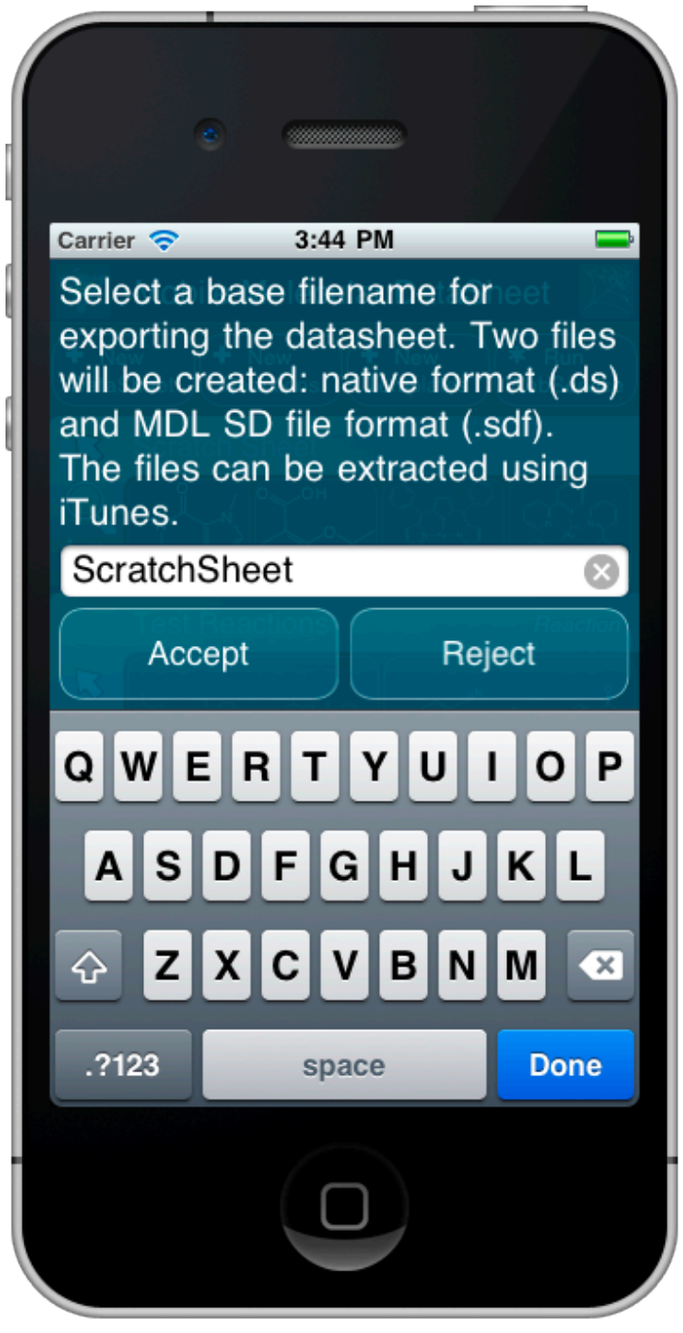
Building services

- 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

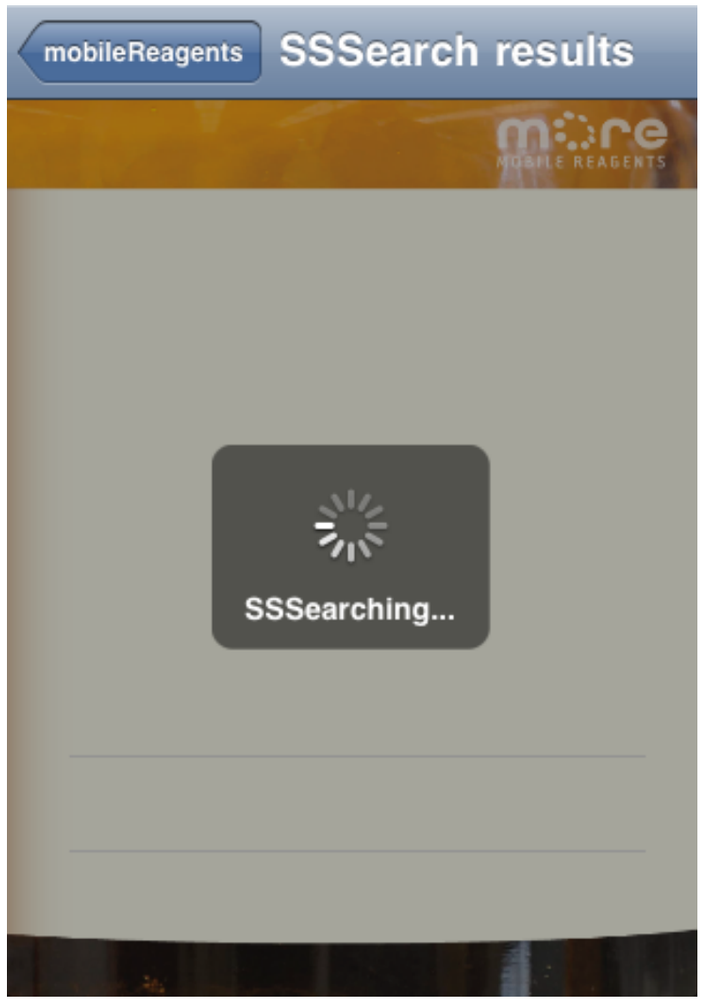
- BlackBerry allows full access to SD card
- iOS allows limited file exchange via iTunes

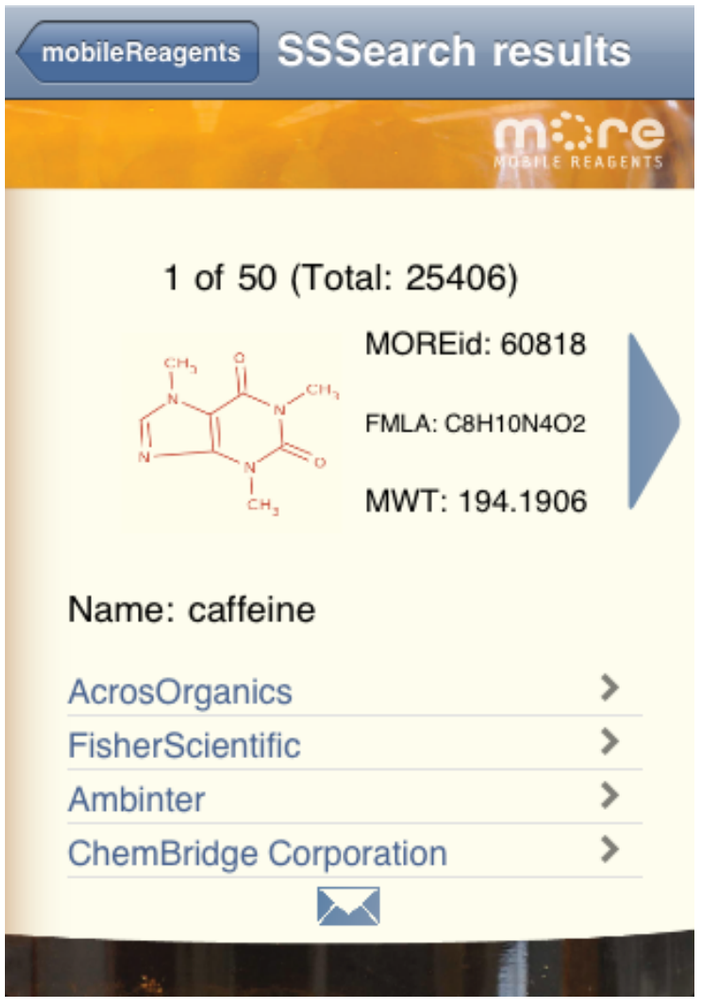


Clipboard and IPC

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

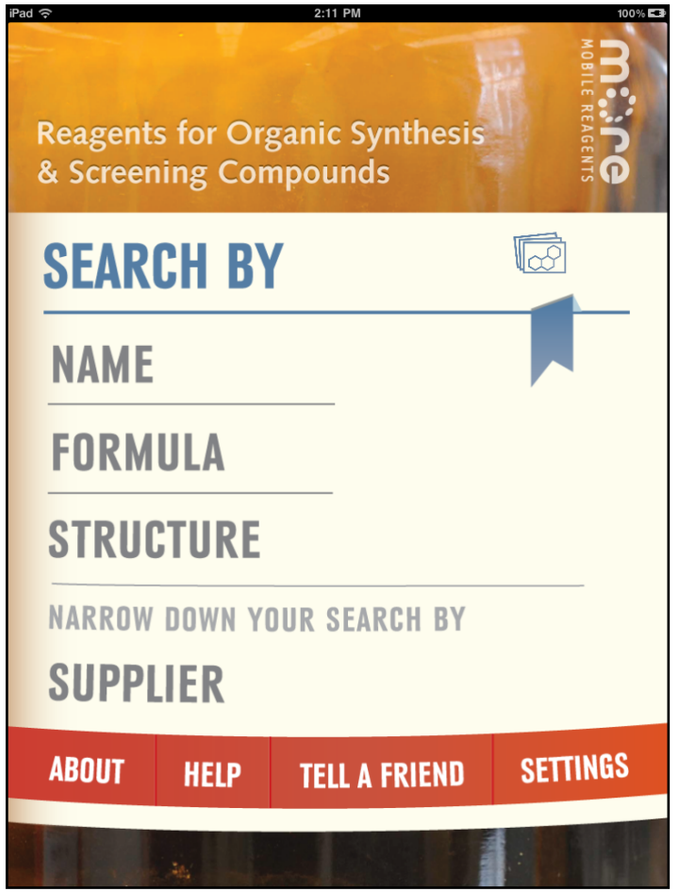
- Can also launch other apps...





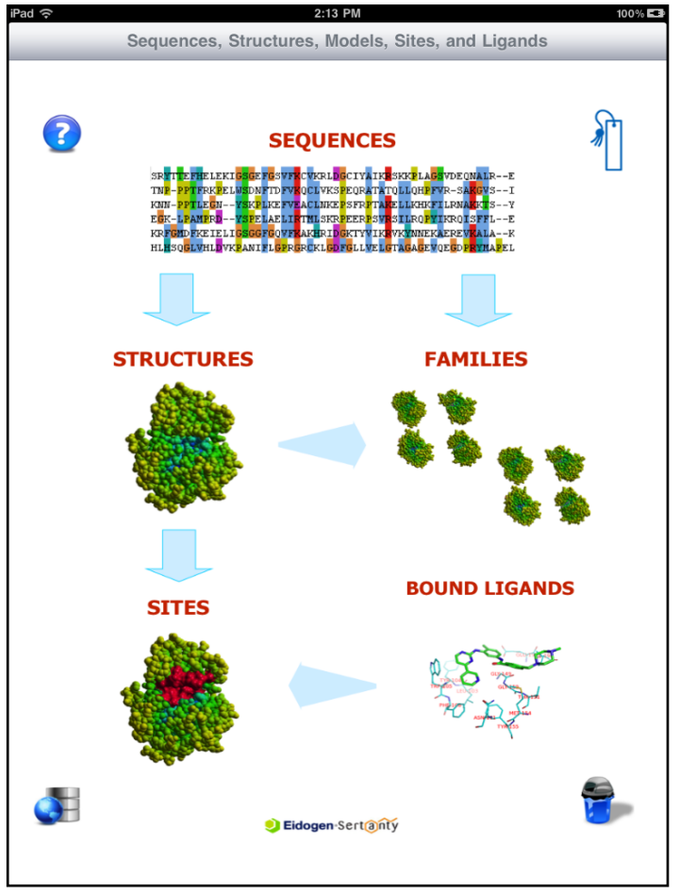
Embedded

- The core tools necessary for a cheminformatics interface have been built...



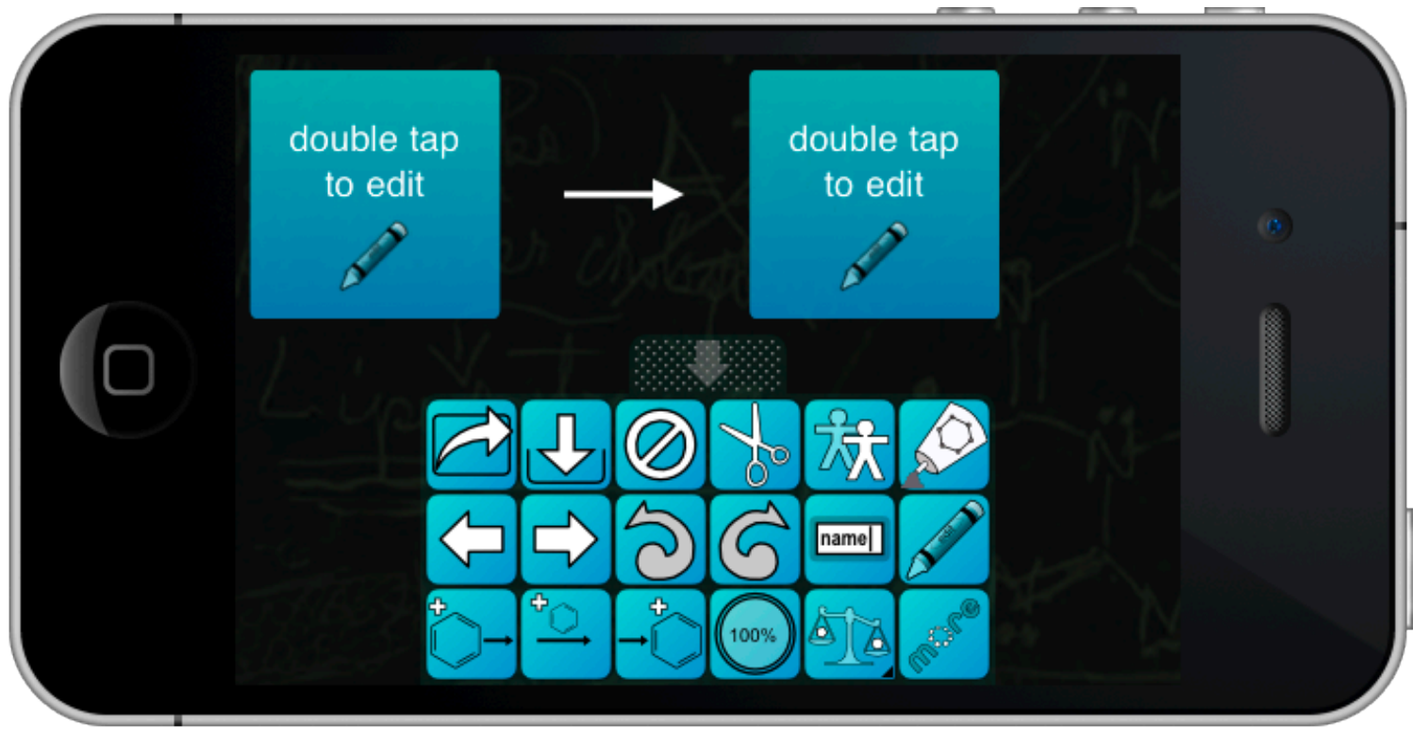
- ... and are available as a linkable library, for iOS devices.

- **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

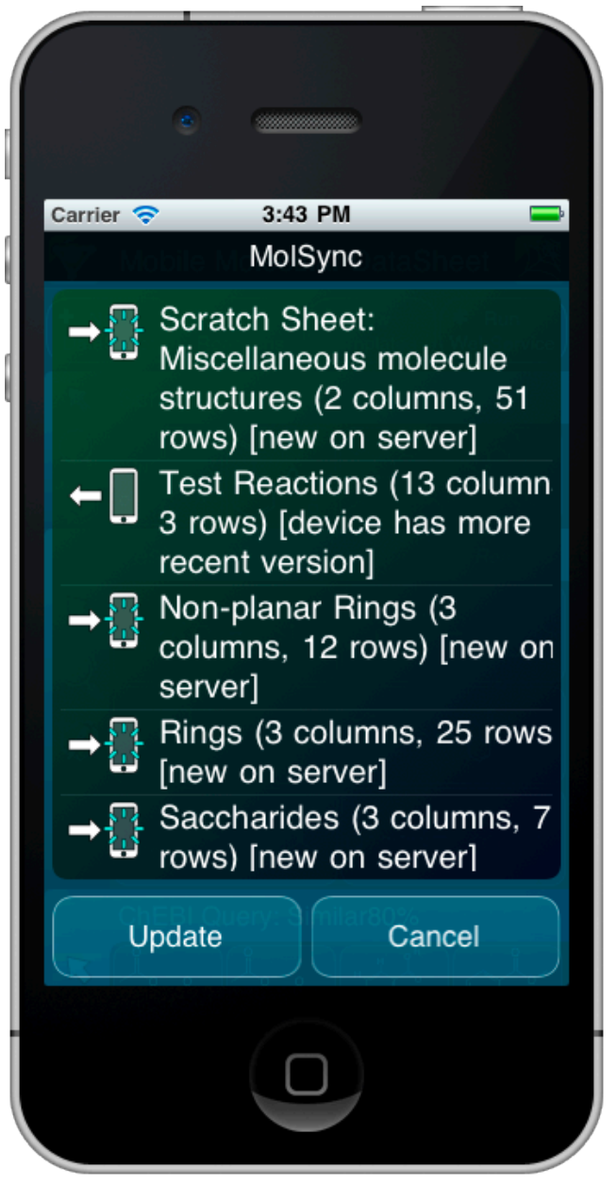
- e.g. custom web services, electronic lab notebook client, specialised tools...

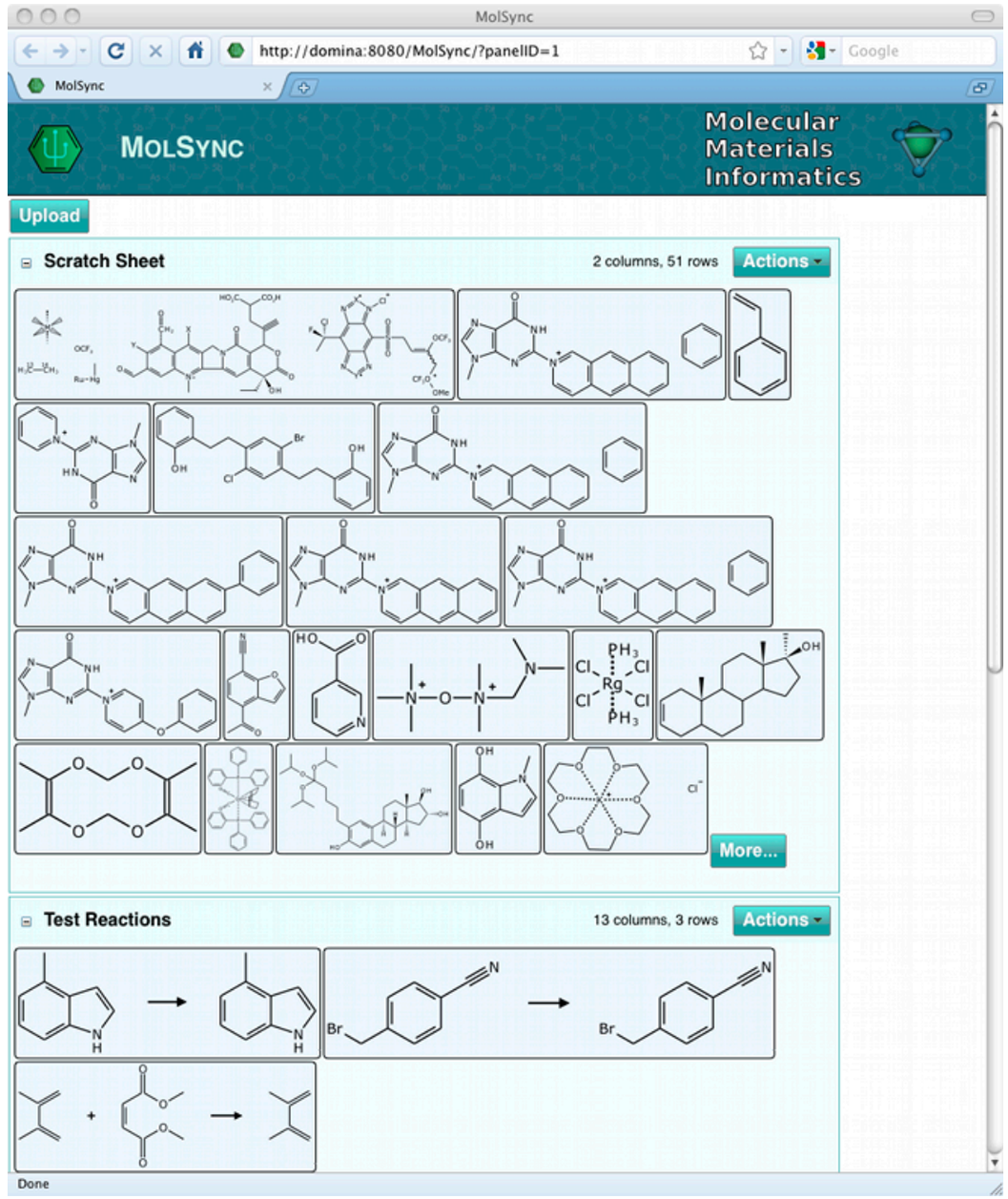
Cloud data

- 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





Other devices

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

- ... 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