Building a mobile app ecosystem for chemistry collaboration

Dr. Alex M. Clark

March 2012

http://molmatinf.com

Mobile apps

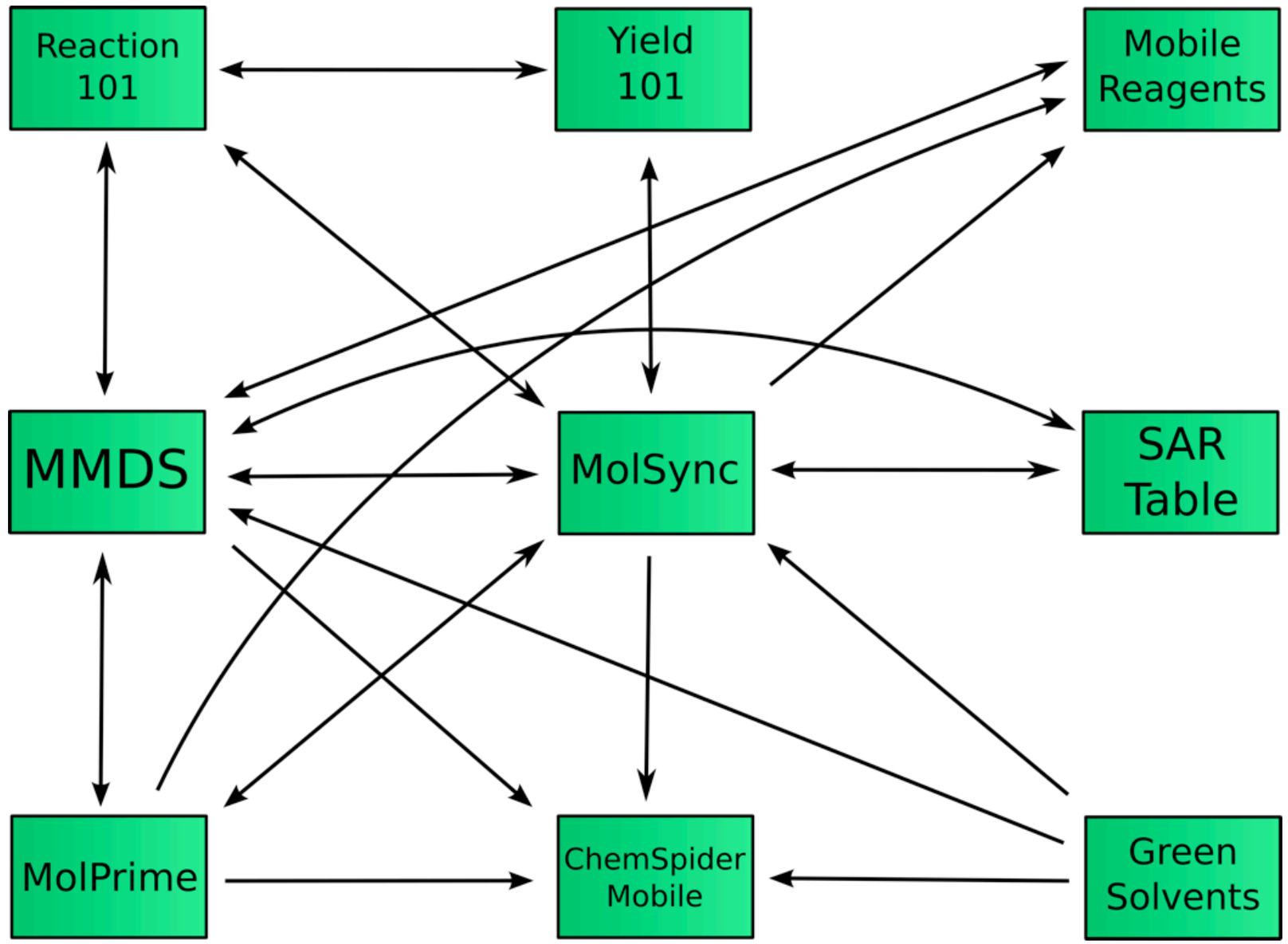
- Most action is for iOS
- Chemistry feature set is becoming very powerful: content **consumption** and **creation**
- **Structure** drawing, **reactions**, **datasheets**
- Access to webservices, calculations, graphics, RPC, social networking, cloud storage

So many apps

- Should be limited in scope, narrow focus...
- ... combine them and they become a toolchest
- Apps can be a major part of a workflow

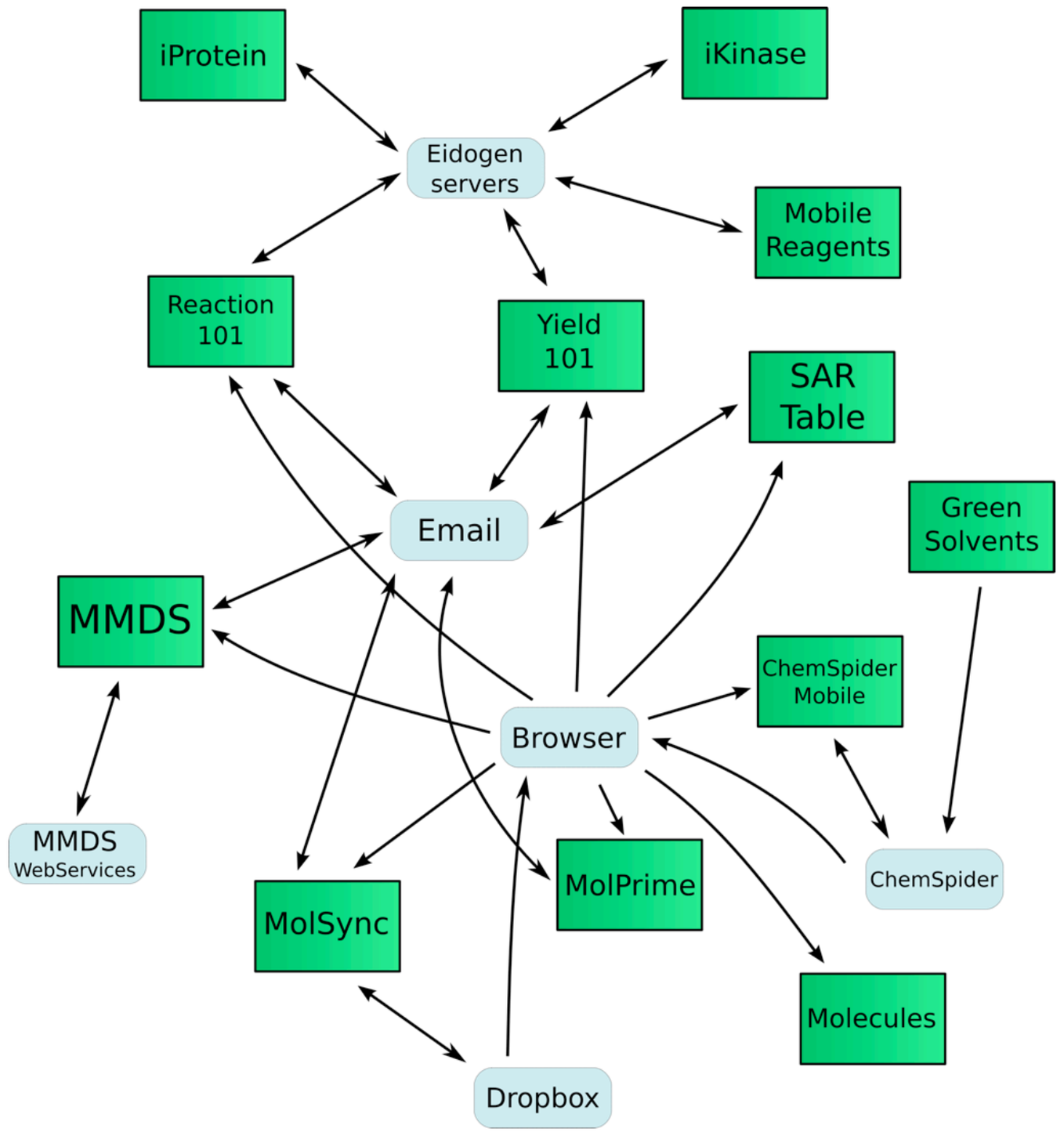
Interprocess comms

- Apps on same device
- Share data:
  - guided
  - unguided
  - clipboard



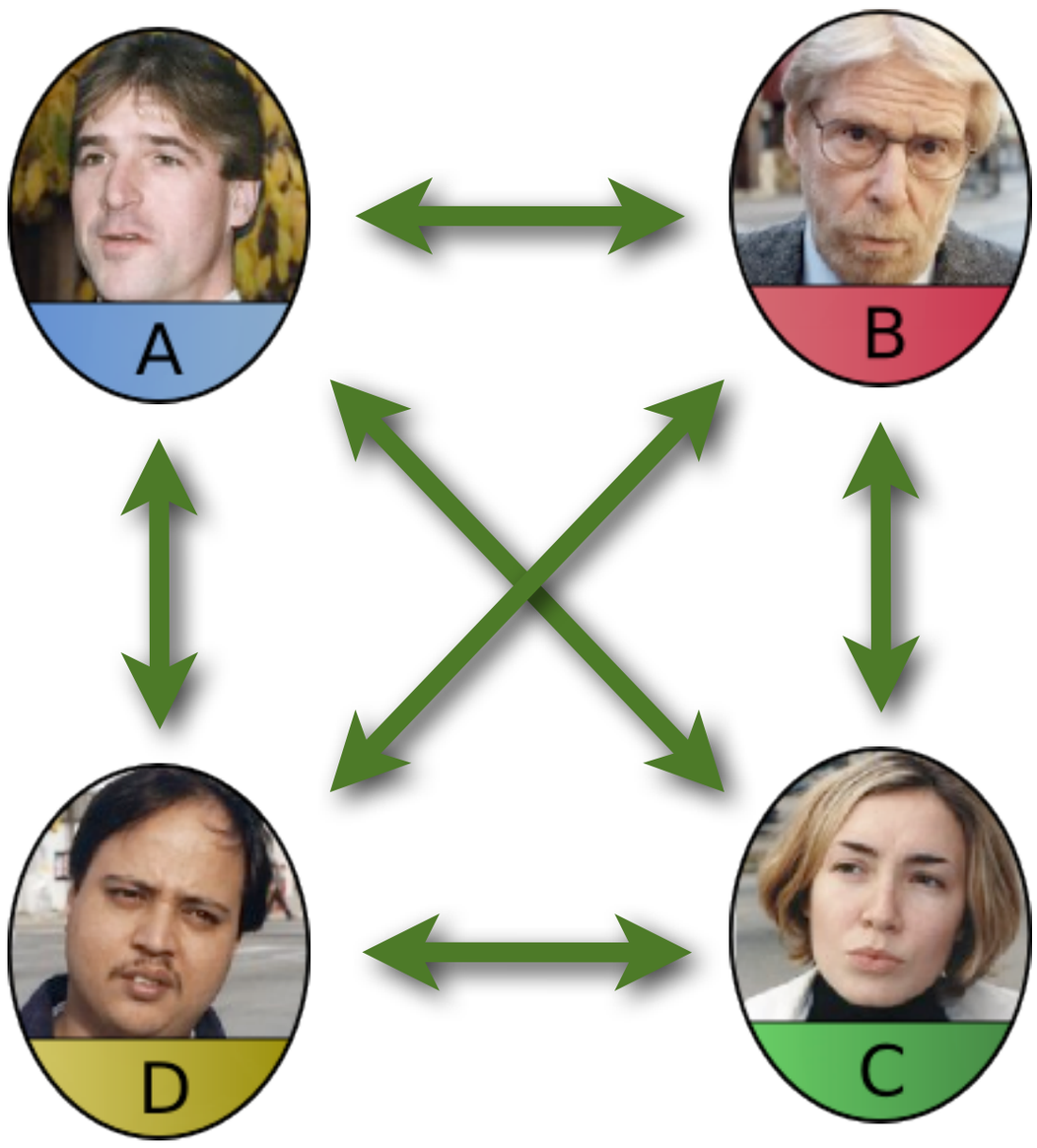
Network comms

- Many different transport mechanisms
  - email
  - file export
  - web access
  - cloud storage
  - client-server RPC
- Heterogenerous platforms



Story

- Illustrating a chemical workflow, involving collaboration between:
  - 4 chemists...
  - ... several devices...
  - ... and lots of apps.



MolPrime+

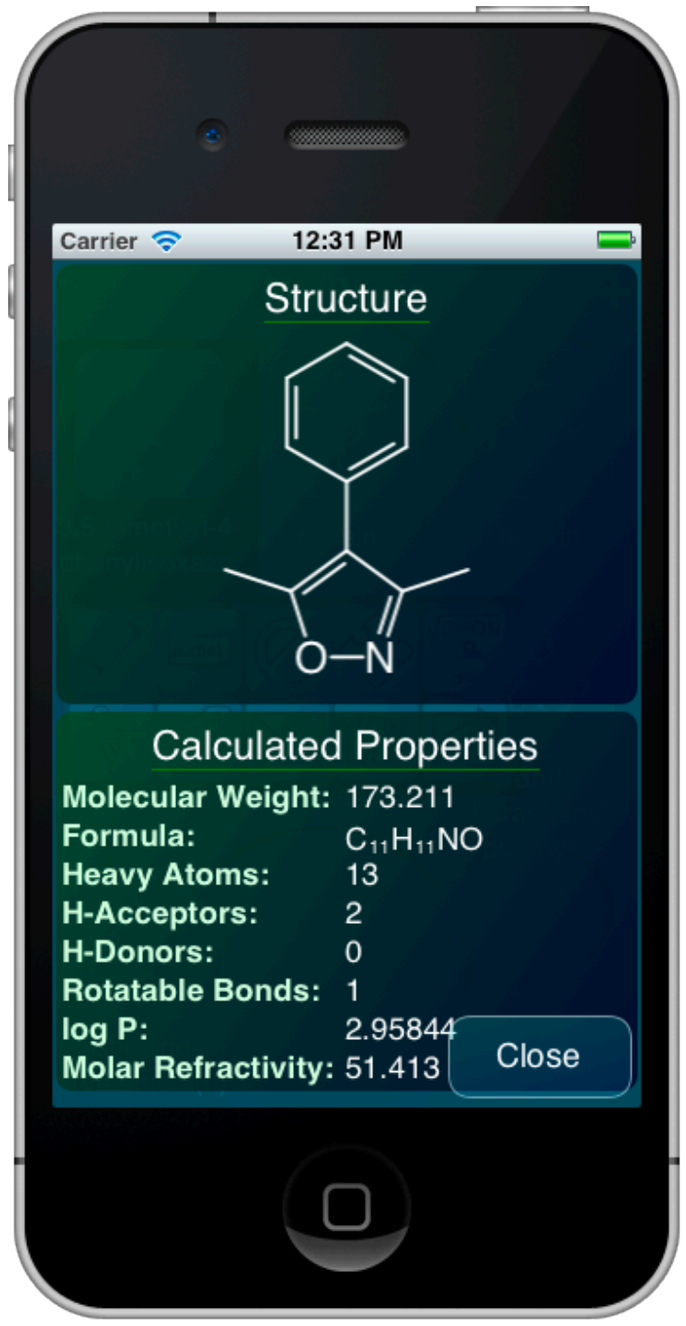
Draw publication-quality structure from scratch, using gestures and templates

bit.ly/GEGonX

Added to molecule collection

Calculated Properties

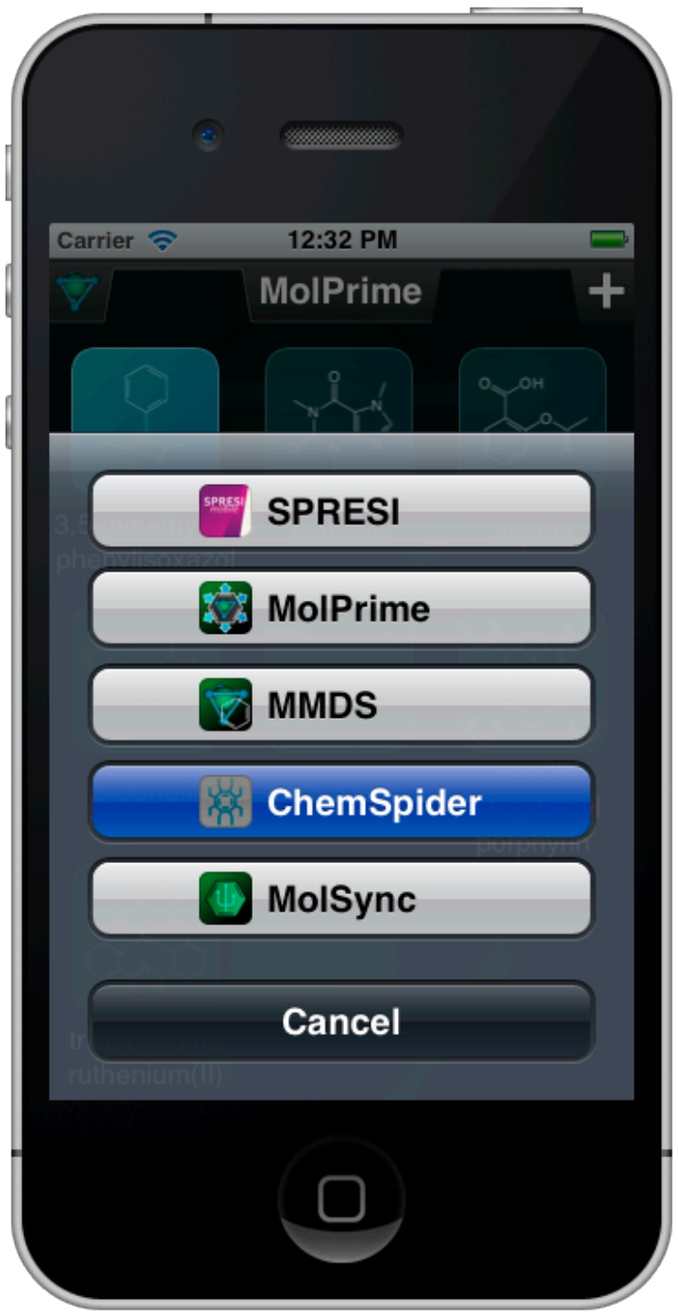
- Access calculated properties



- Simple properties calculated within the app

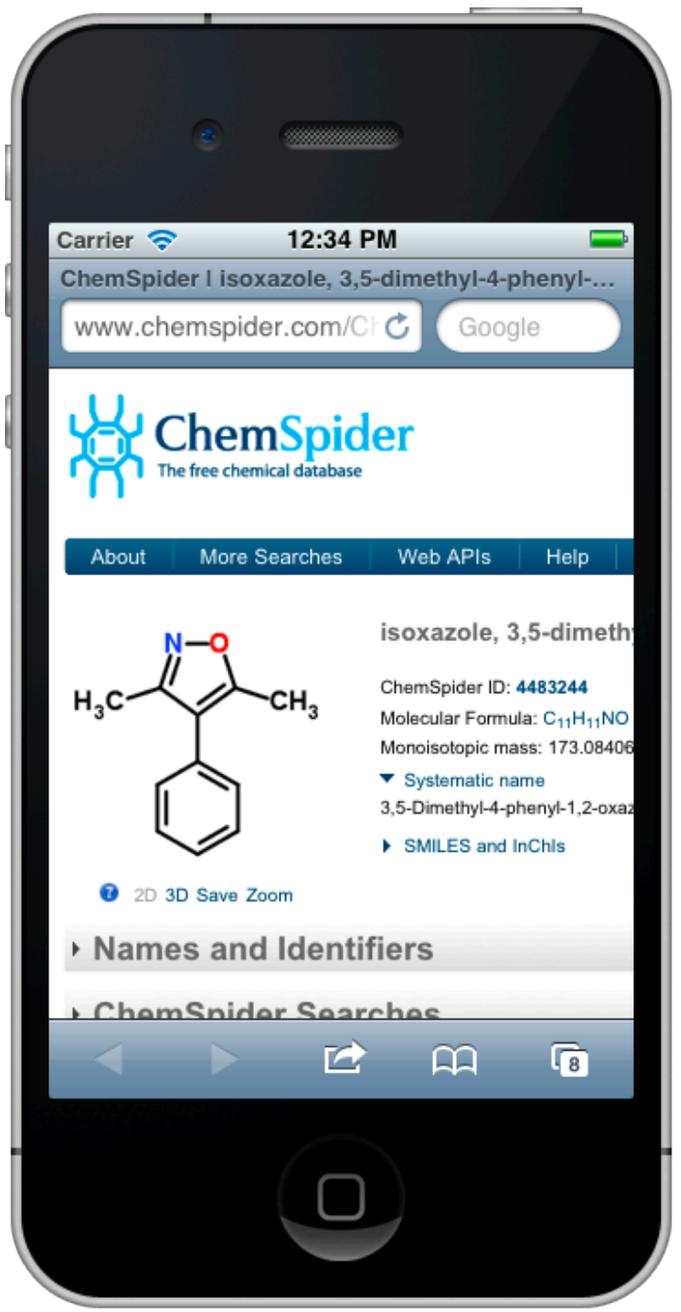
- Complex properties use **RPC** call to web service (log P, MR)

ChemSpider Mobile



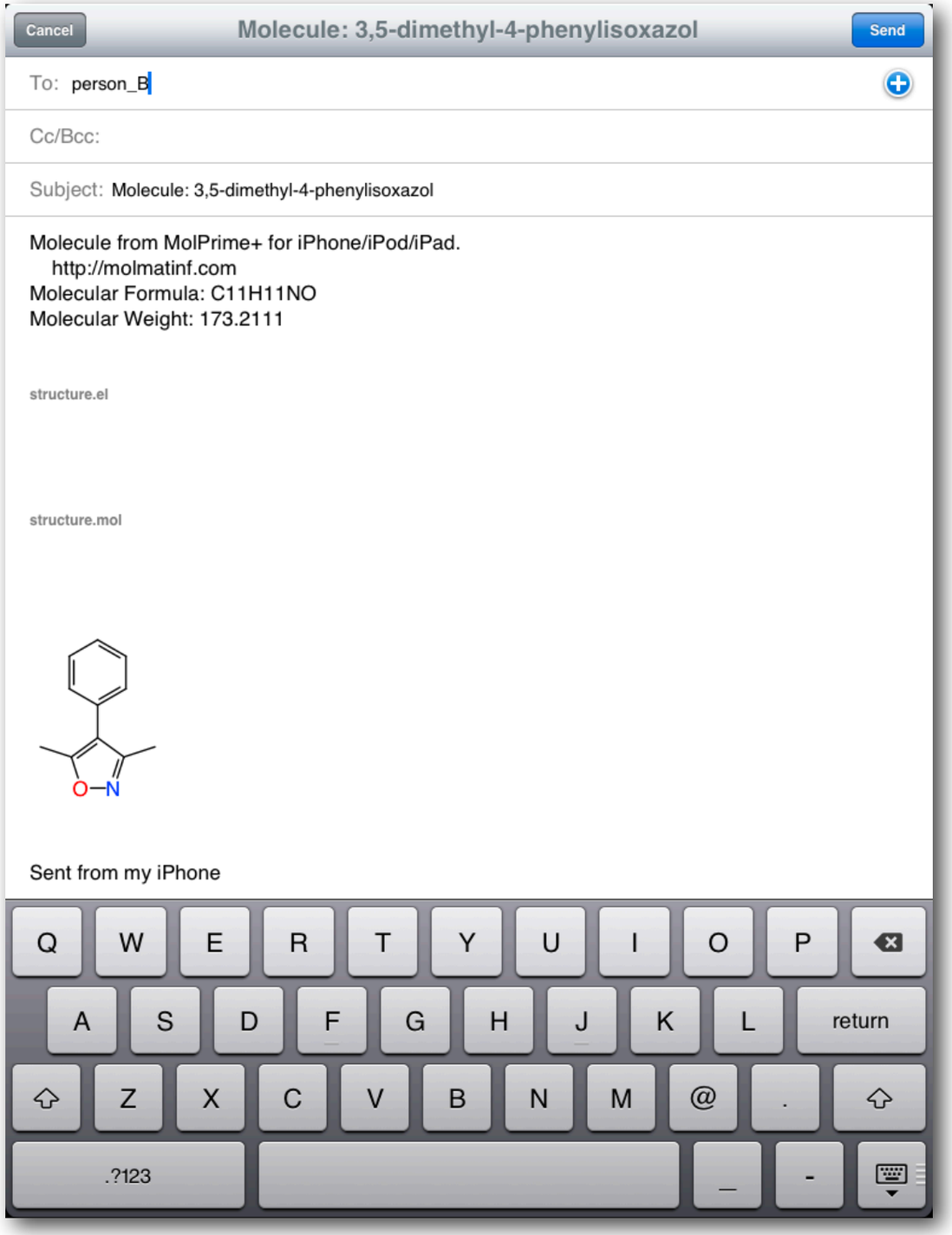
Use **Open With** to send the structure to the *ChemSpider Mobile* app

Search and open the web page



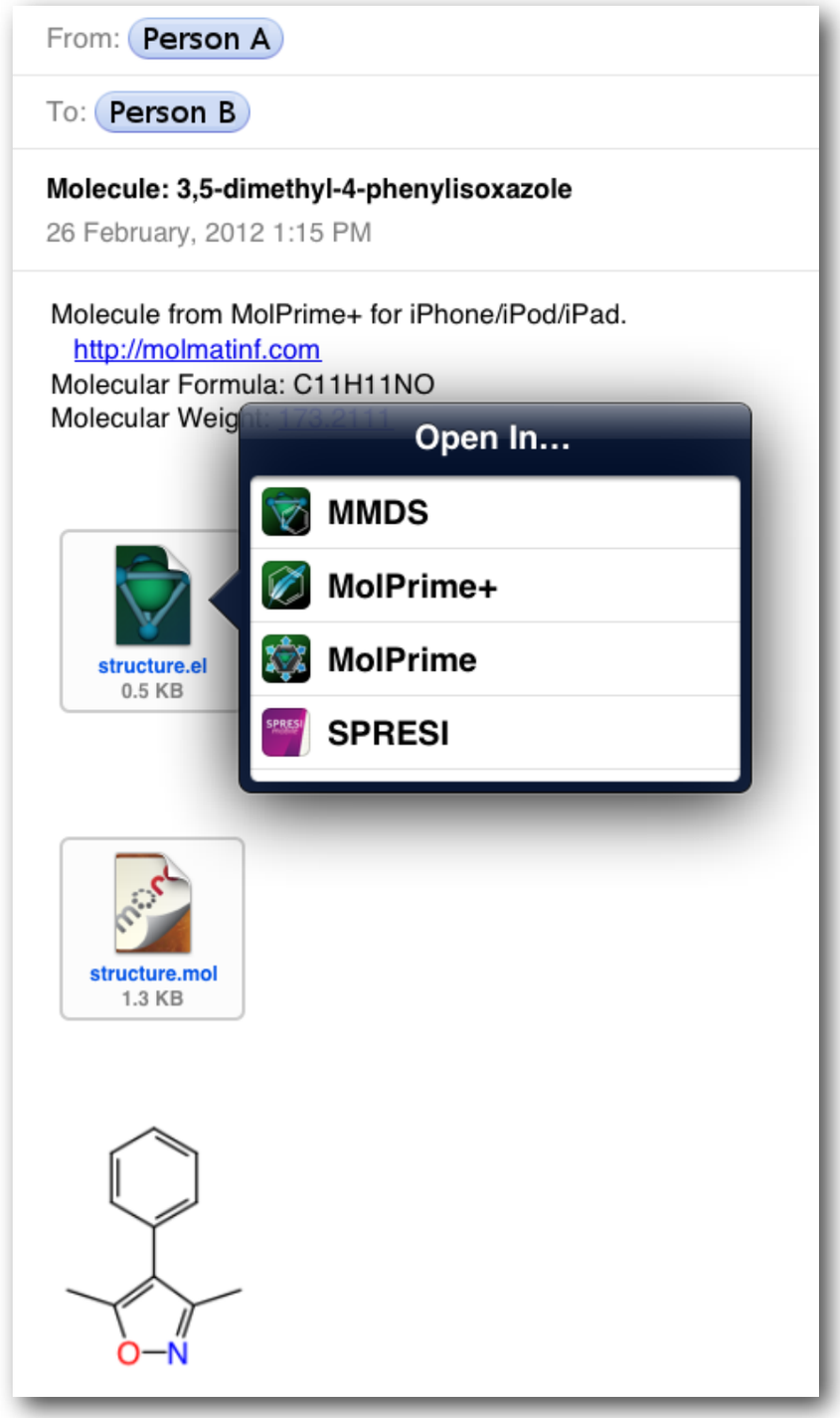
Email

- Prepare an outgoing email
- Includes structure data, and prepared image
- Send to **Person B**



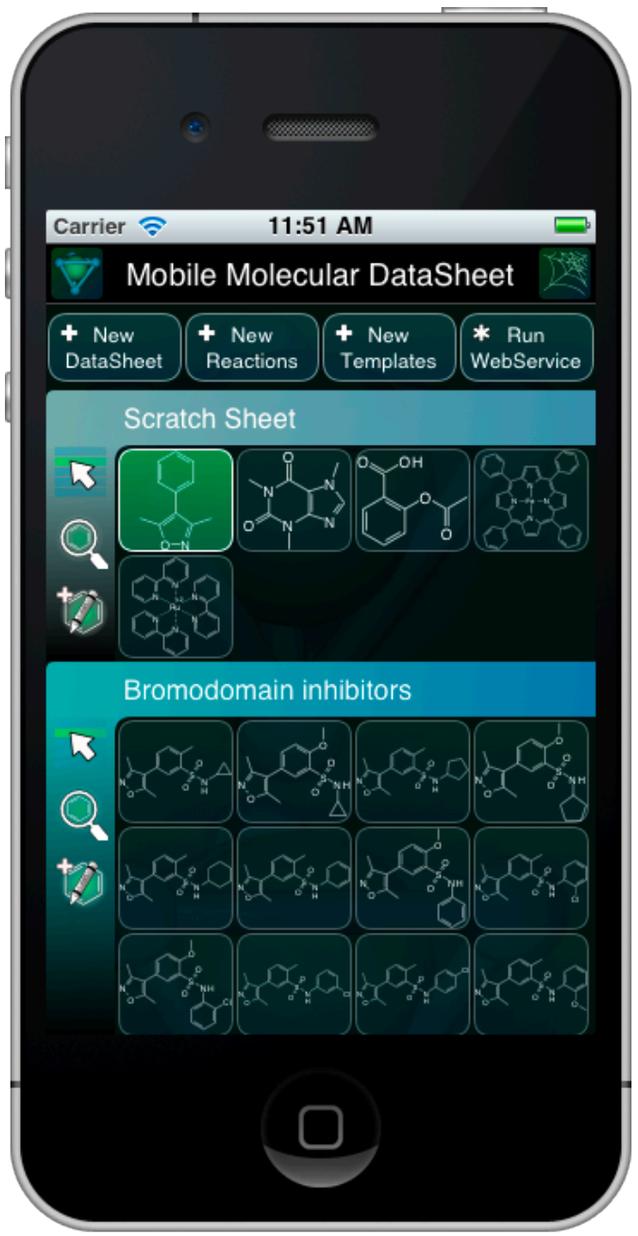
MMDS

- Email offers a list of apps that can handle each attachment
- Person B is a power user...
- ... opens the structure file with the *Mobile Molecular DataSheet*



MMDS

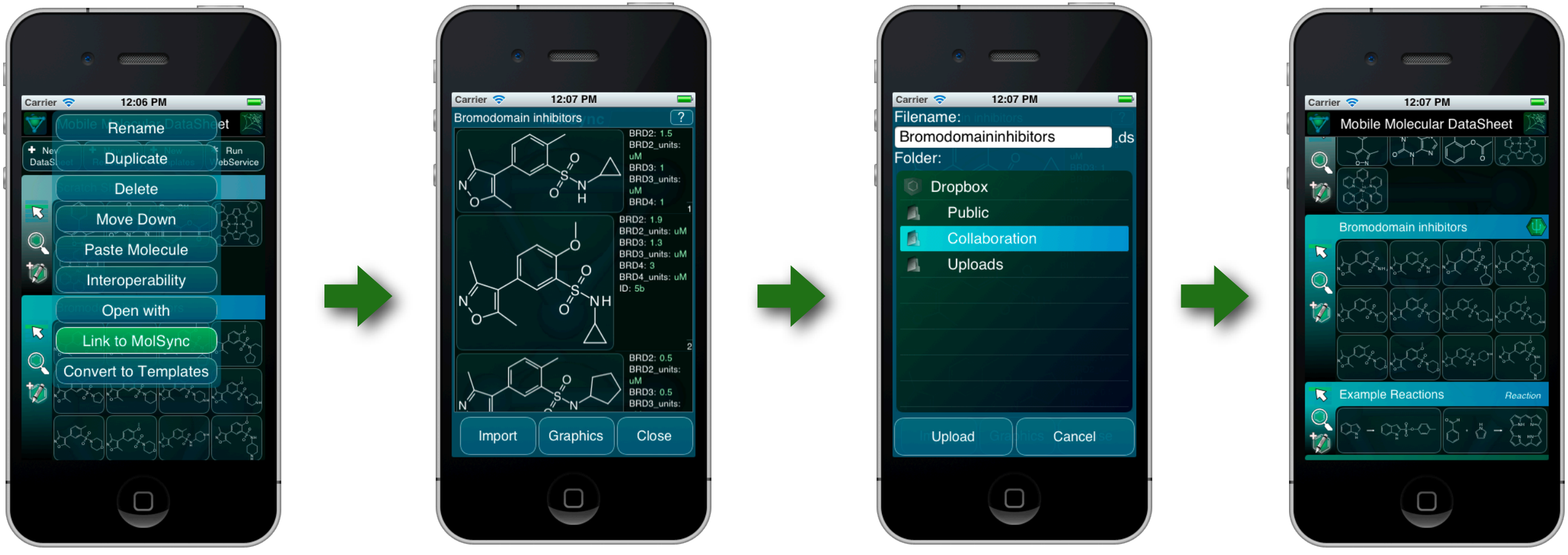
Mobile Molecular DataSheet



Structure is prepended to *scratch sheet*

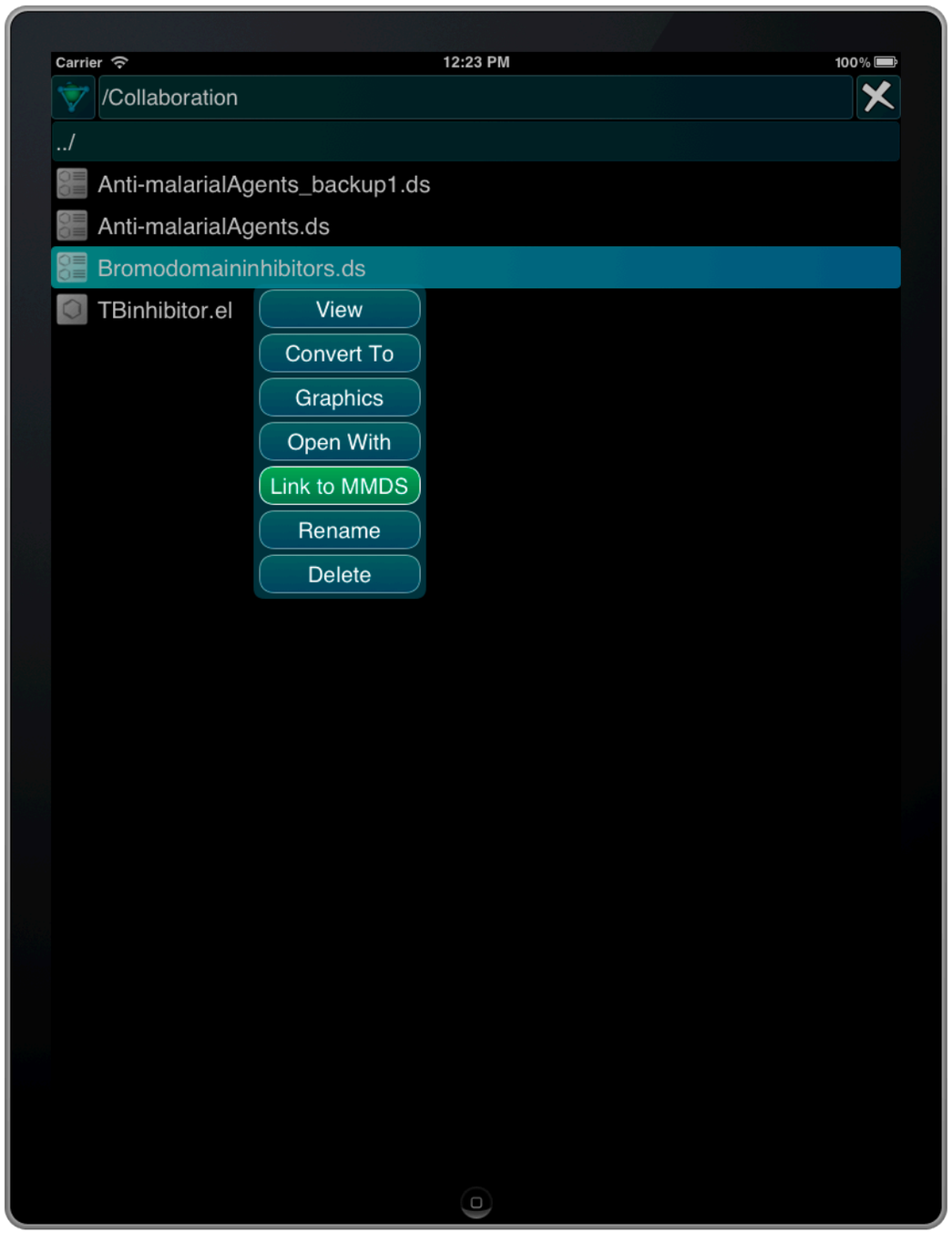
Can copy/paste into a datasheet of *bromodomain inhibitors*

MolSync



- Communicate with *MolSync*
- *Upload to Dropbox*
- *Create association*

MolSync



- **Person C**, an experimentalist, accesses shared folder from an iPad
- Opens datasheet with *MMDS*
- Creates shared association

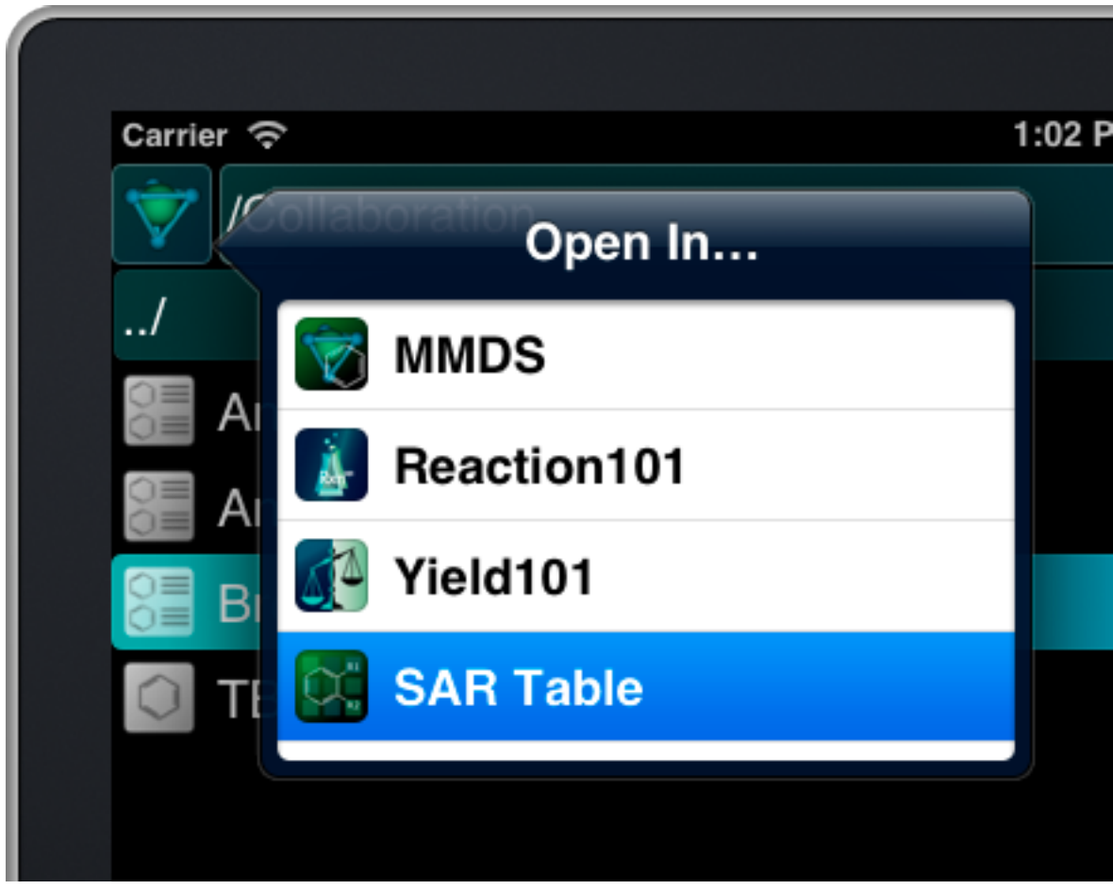
MMDS

- Runs the experiment, measures the activity values
- Enters the data fields using *MMDS*
- Resyncs the file via *MolSync*...
- ... uploads modified version to *Dropbox* folder

MolSync

- **Person B** uses *MolSync* to view the datasheet in the shared folder

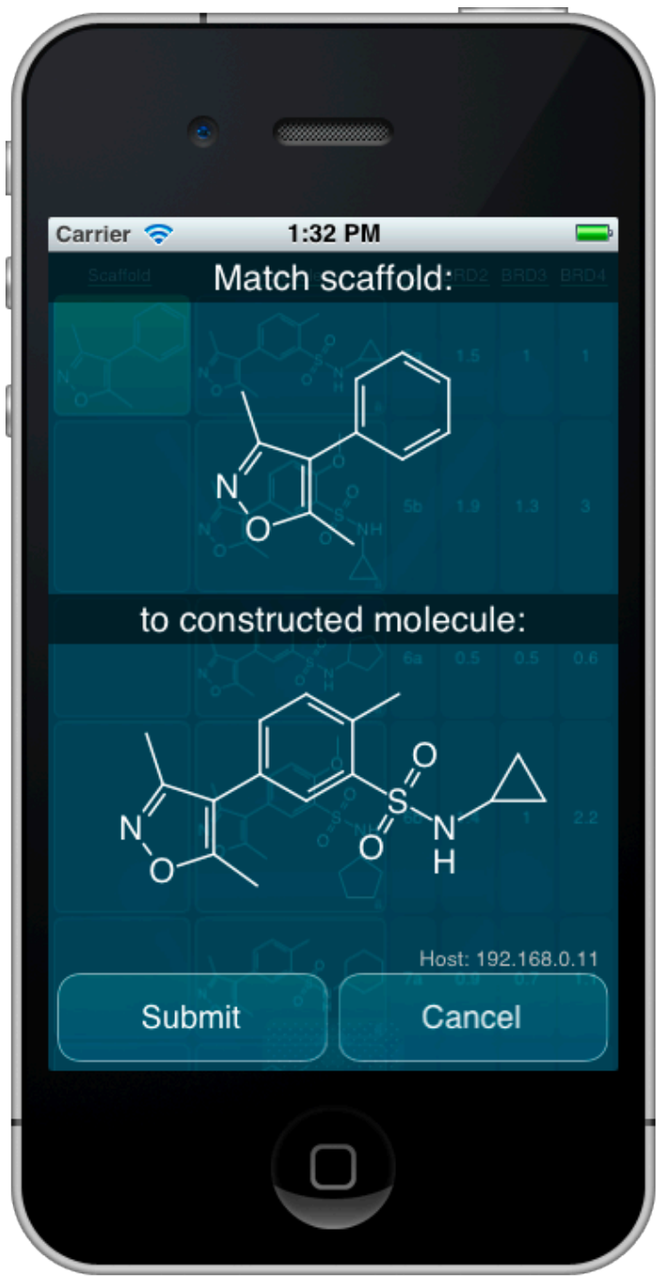
- Series is complete: open the datasheet with the *SAR Table* app...



SAR Table

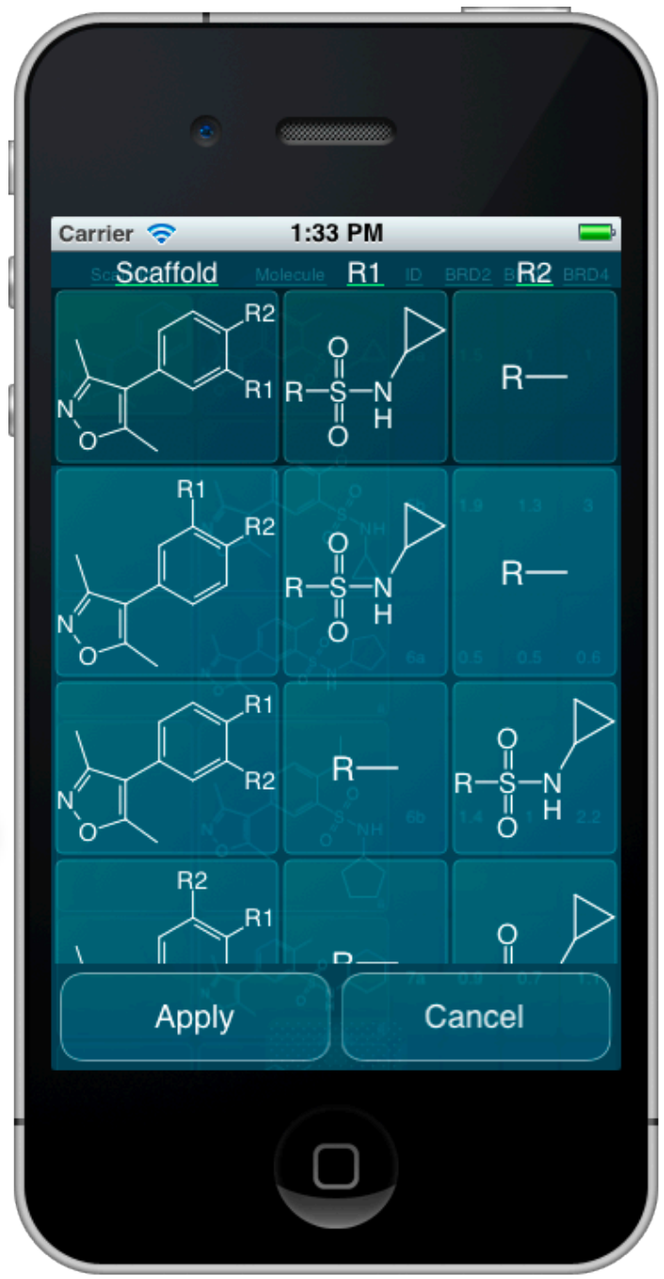
- Imported content has *construct* molecules
- Copy first molecule into *Scaffold* field
- Trim off substituents
- Use the **Match** feature...

SAR Table



Initiate the match: calculation is done by *remote procedure call*

A variety of possibilities: select the preferred one

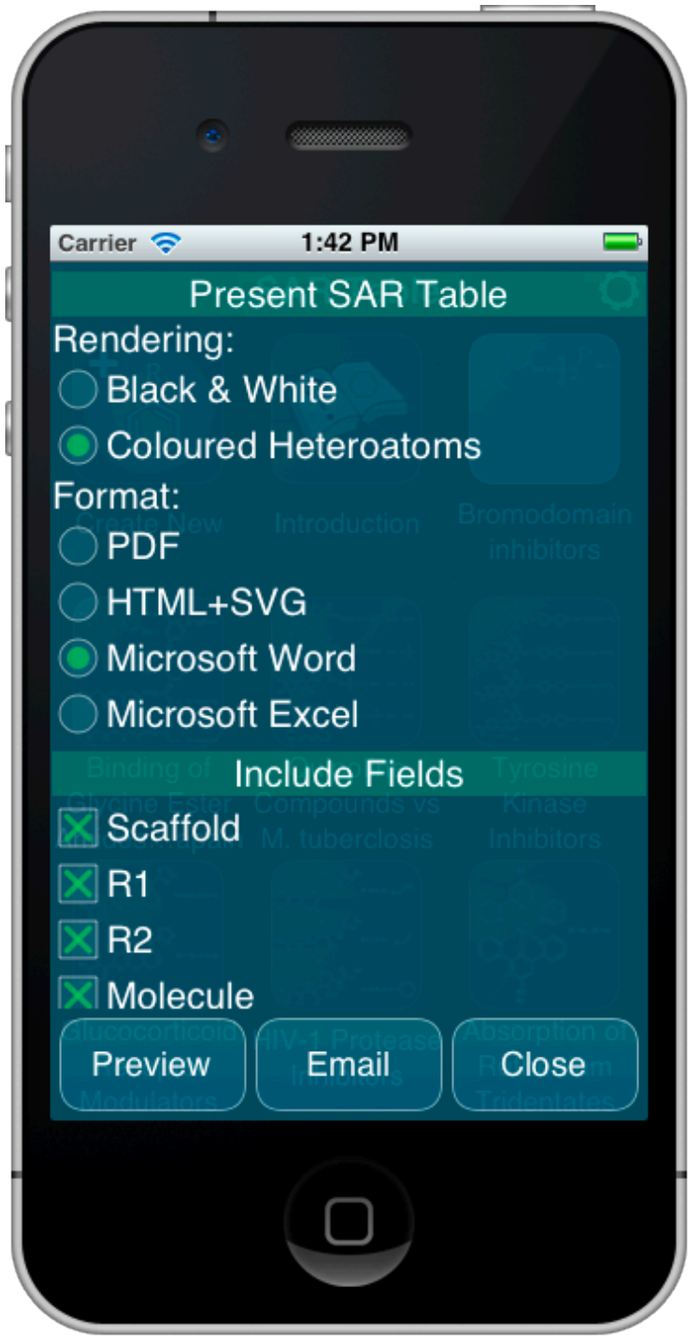


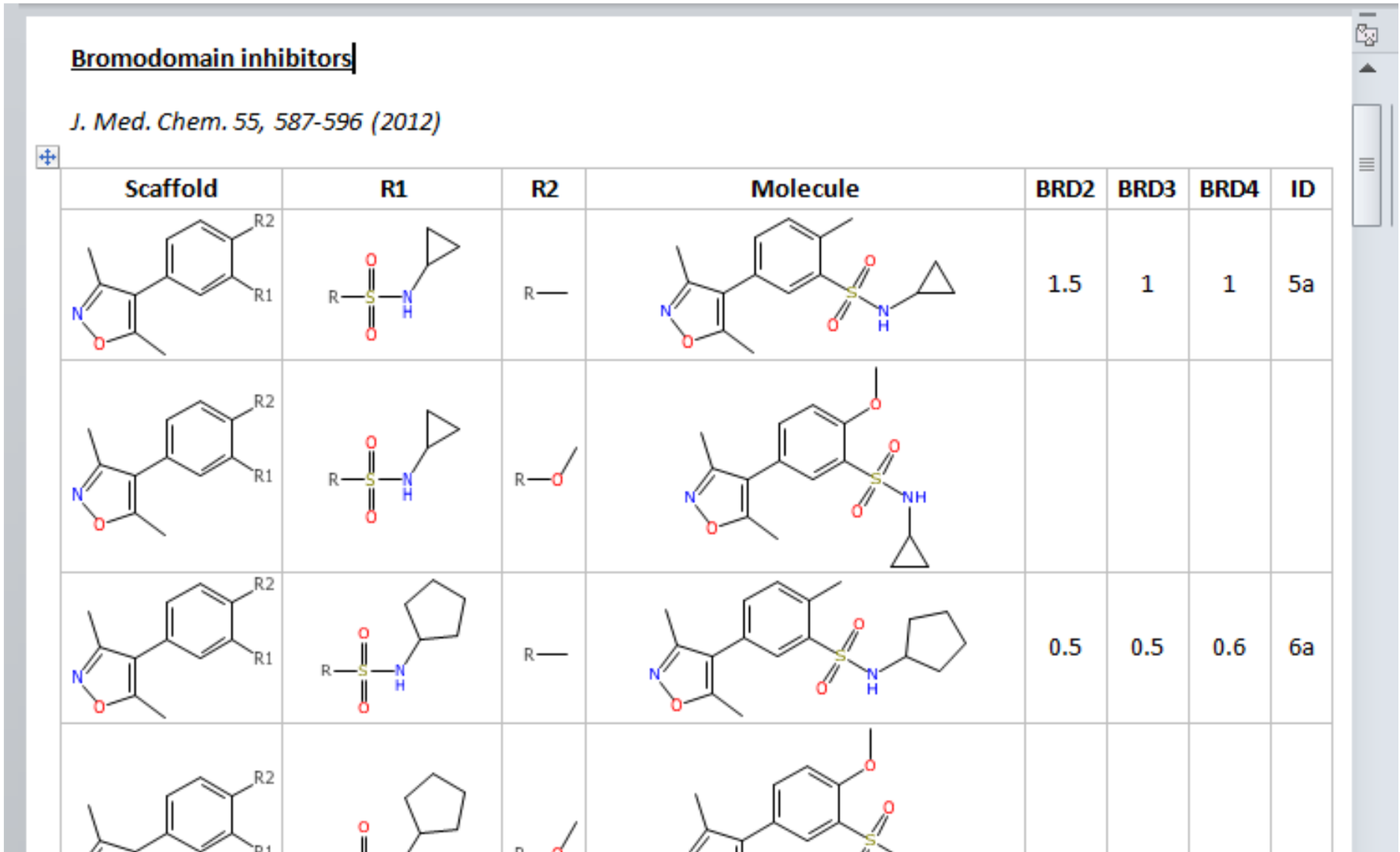
SAR Table

- Scaffold has been decorated
- **R1** and **R2** columns defined
- Rinse and repeat
- Scaffold matching uses previous assignments to influence suggestions

SAR Table

- Can export the table via email as MS Office documents (.docx, .xlsx)
- Structures use **vector graphics**





Bromodomain inhibitors

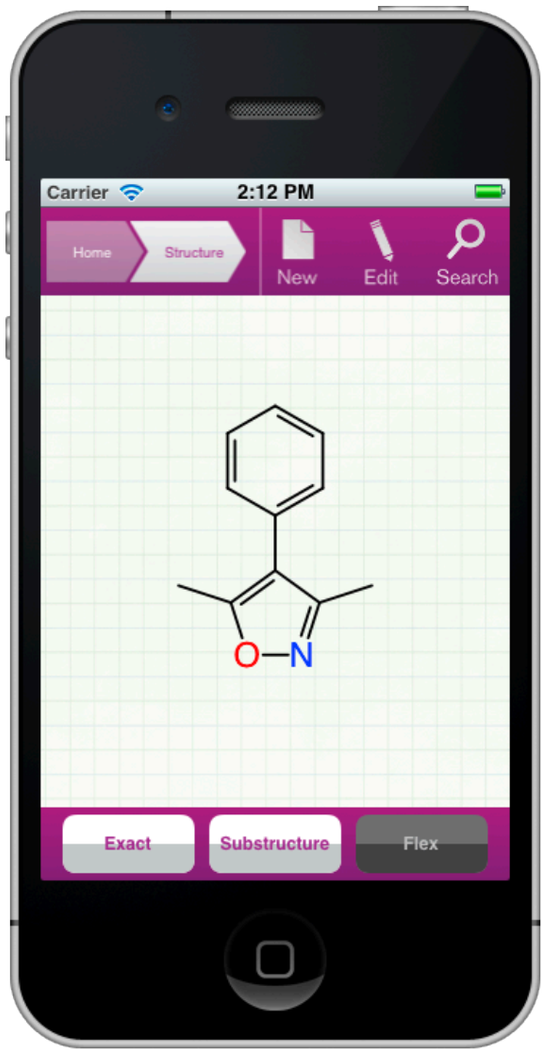
J. Med. Chem. 55, 587-596 (2012)

Scaffold	R1	R2	Molecule	BRD2	BRD3	BRD4	ID
				1.5	1	1	5a
				0.5	0.5	0.6	6a

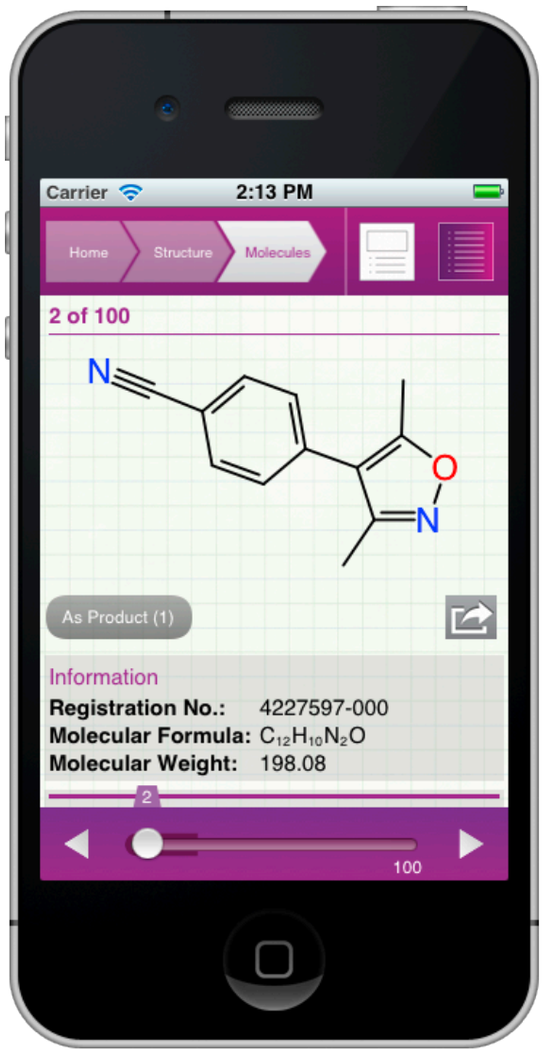
SPRESI*mobile*

Want to illustrate a representative synthesis: search for the common fragment using SPRESI

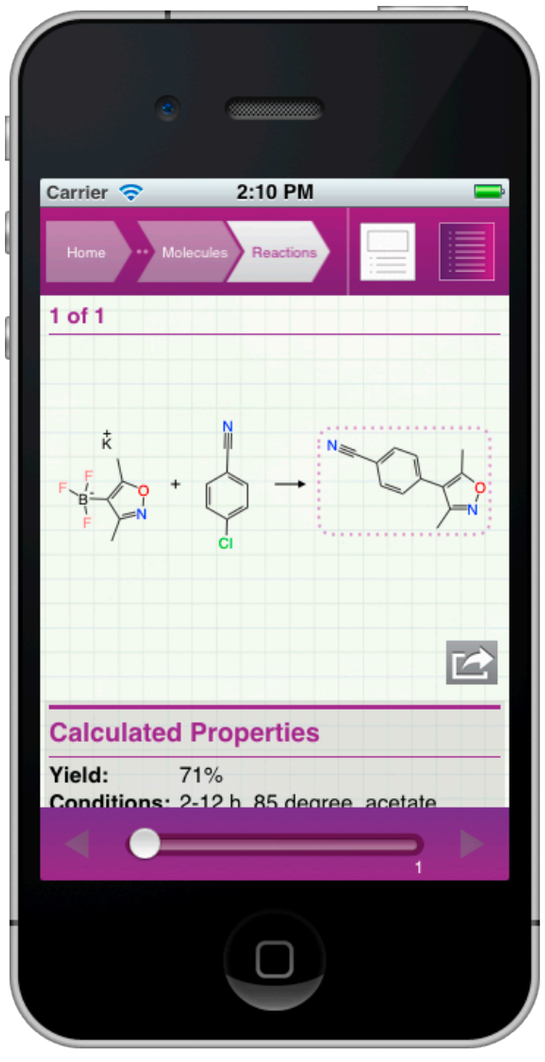
Open With



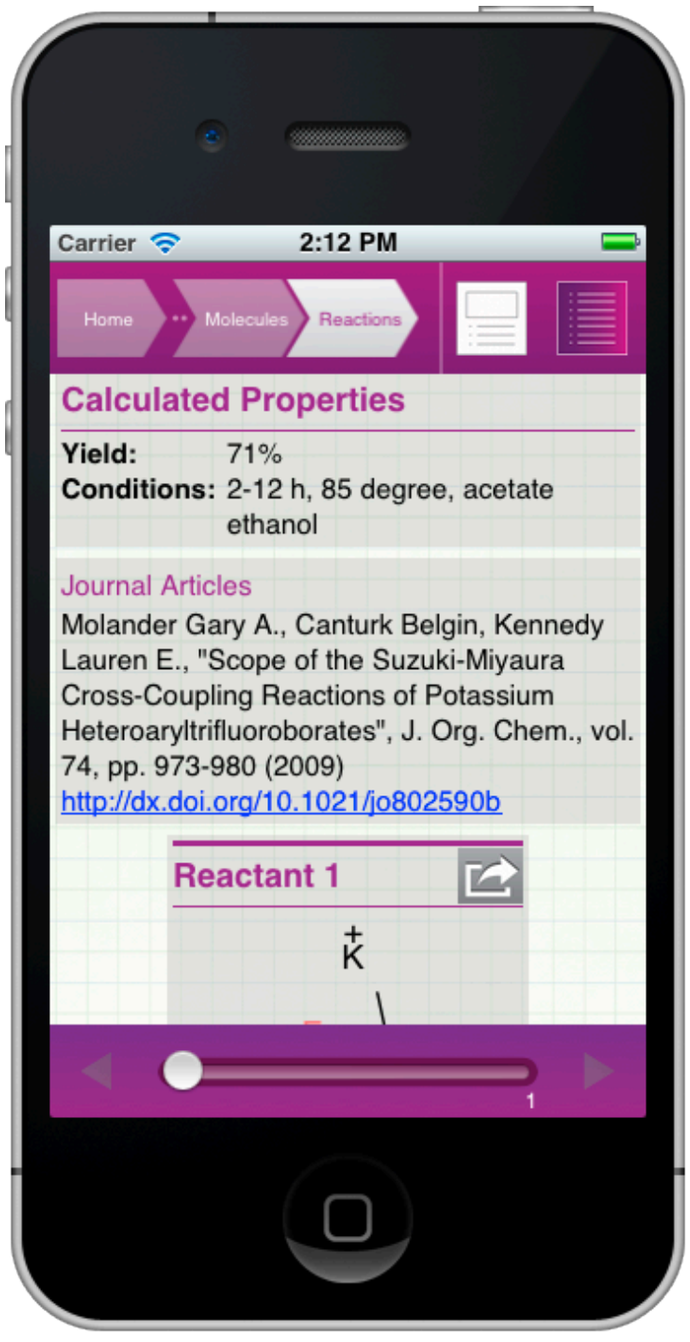
Search



As Product

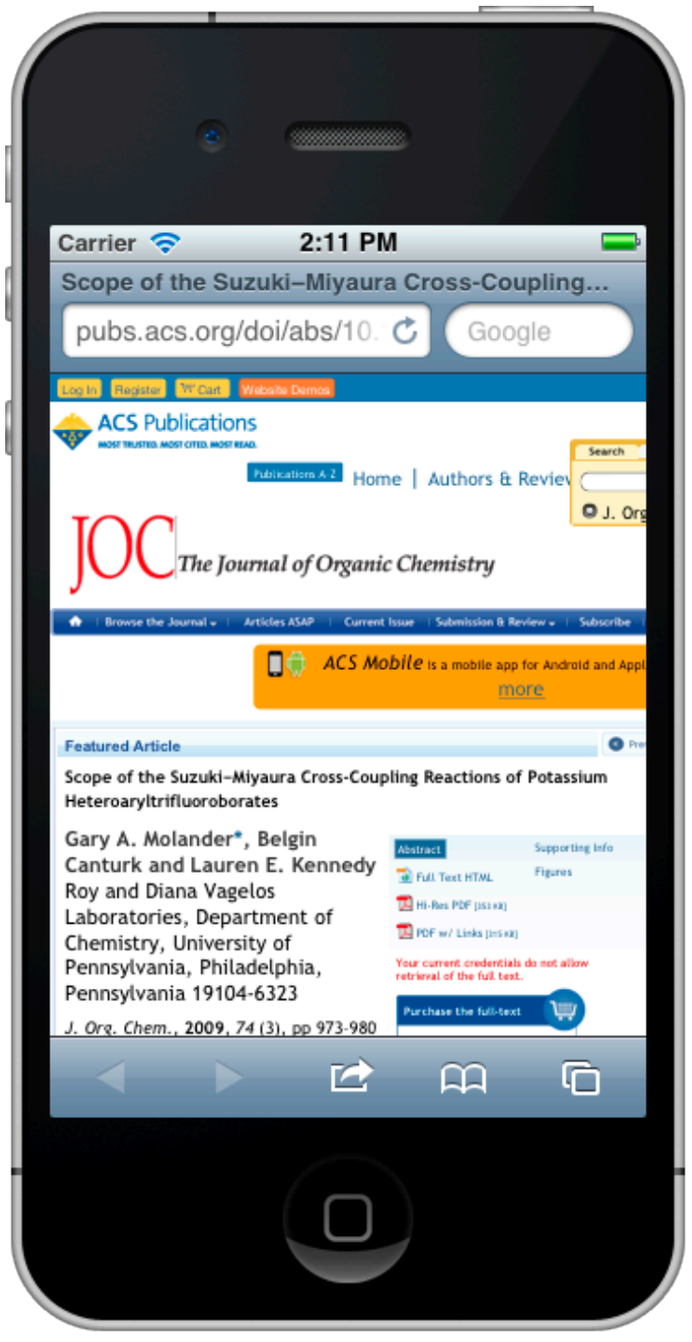


SPRESI*mobile*

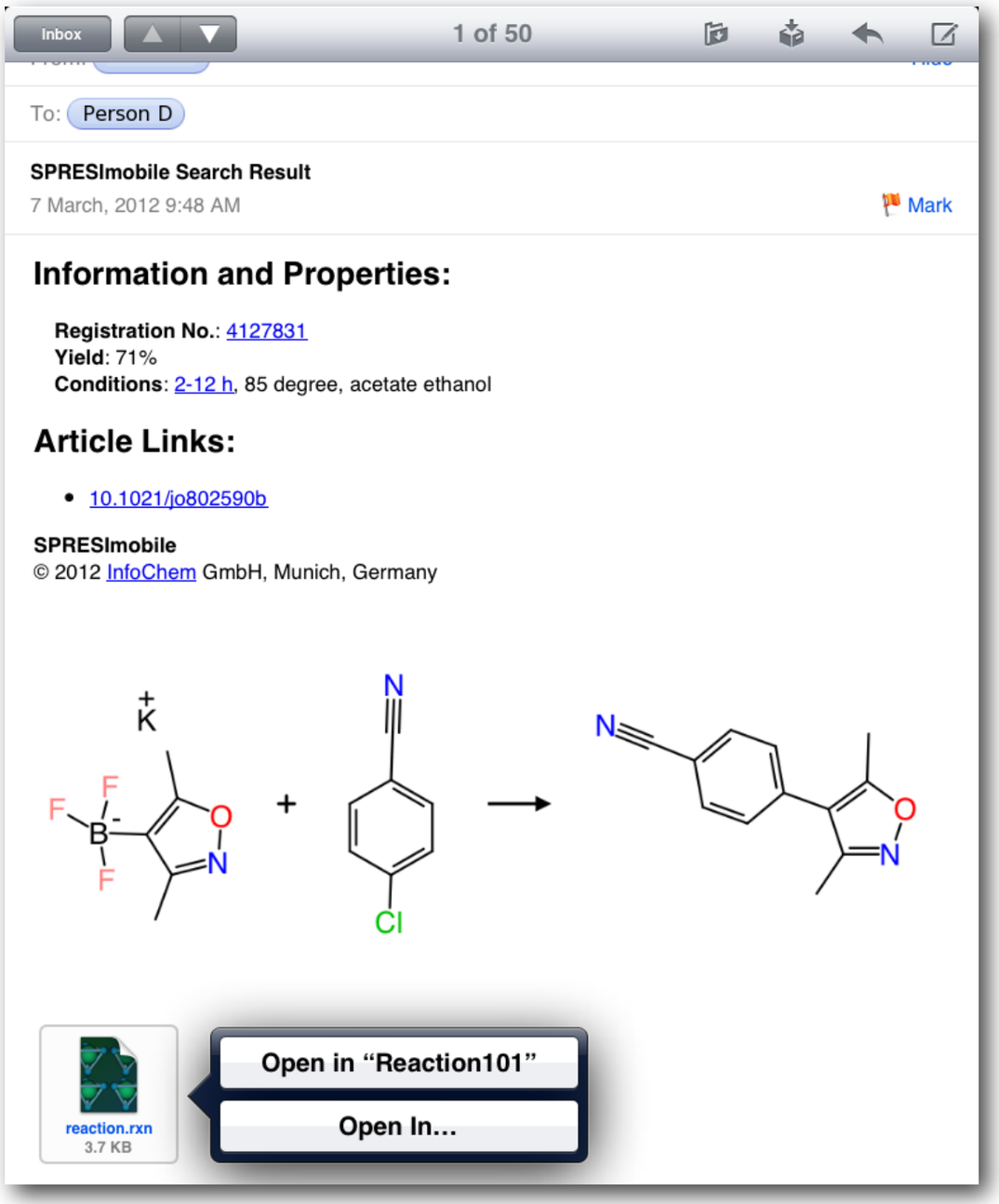


All content links to the scientific literature

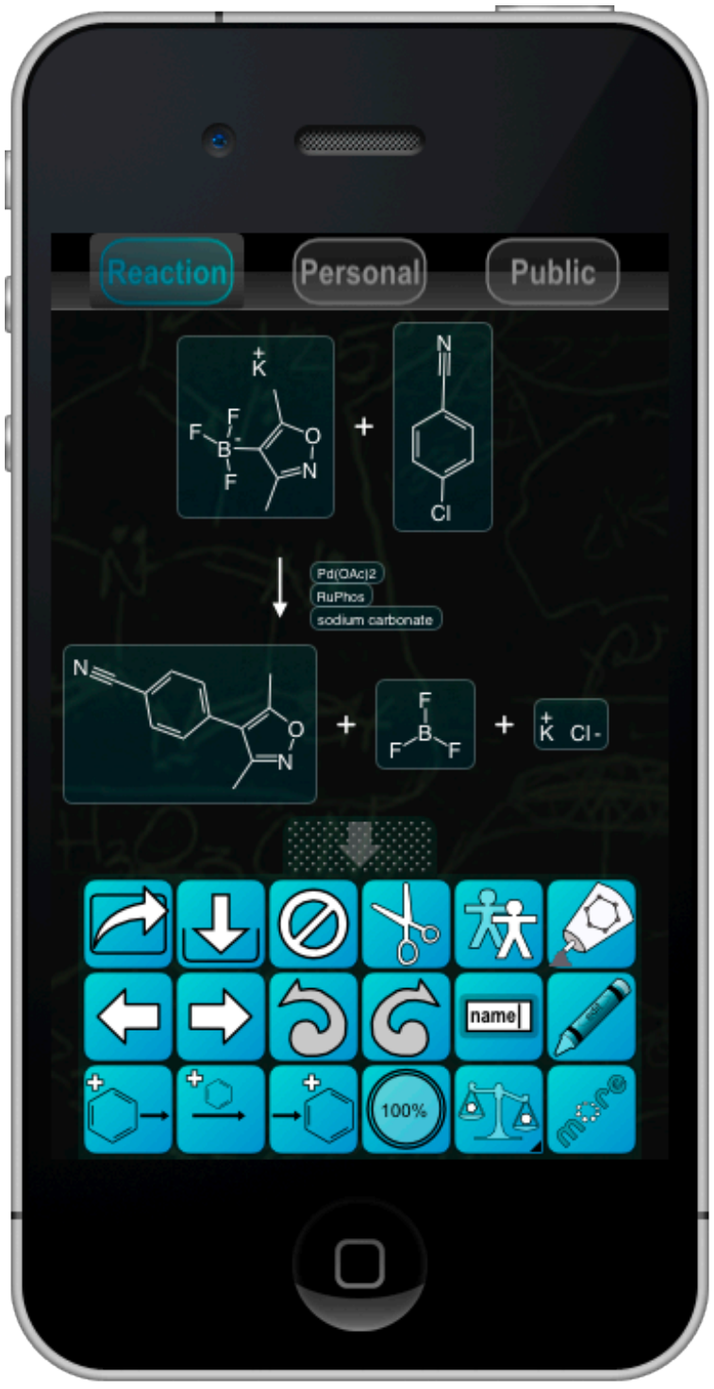
Can access the journal article with one tap



Reaction101



- **Person D** opens email with *Reaction101*
- Balance, add reagents, store



Yield101

- Opens *Yield101* and accesses personal reactions to obtain the balanced reaction template

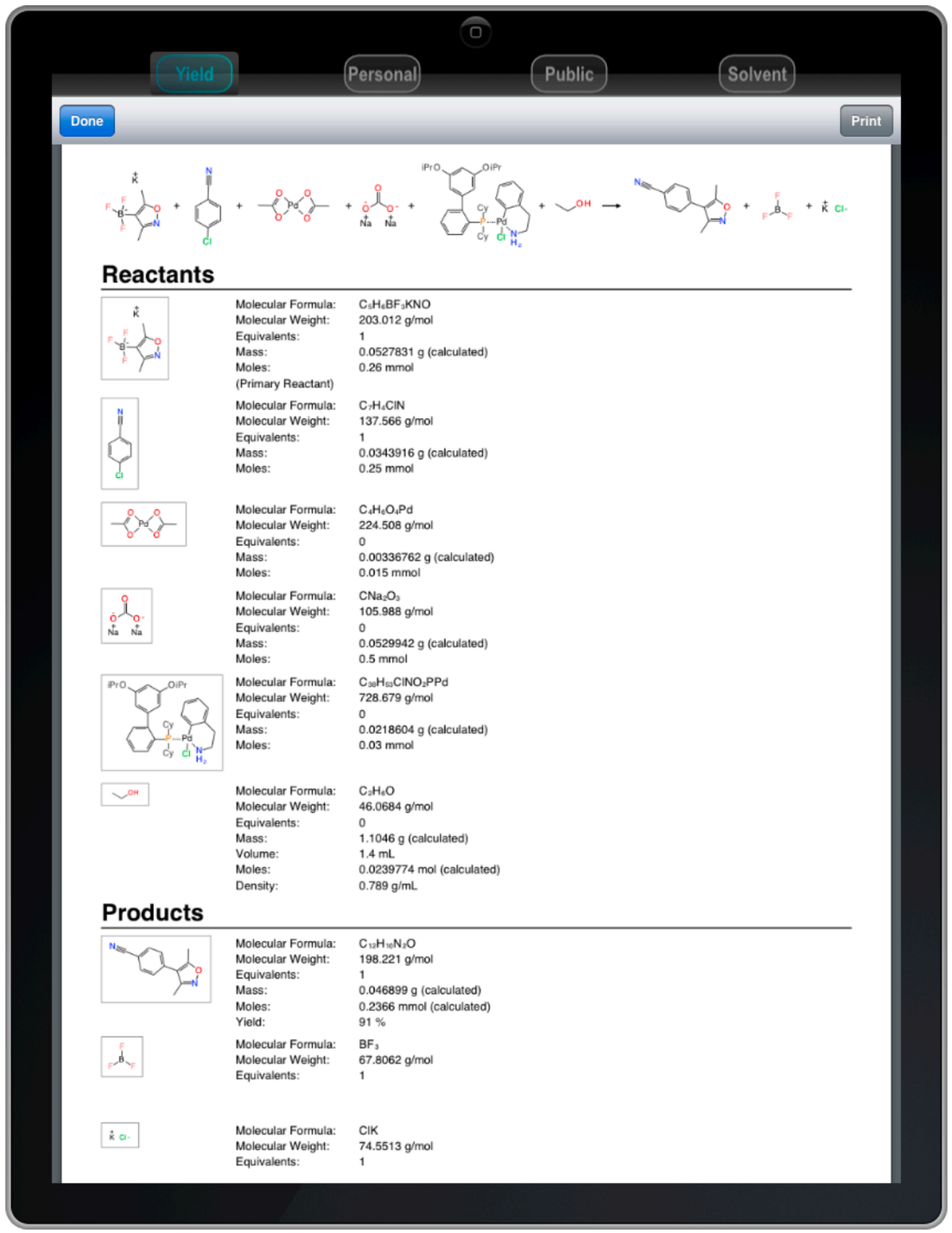
- Fills in quantities, adds solvent, checks availability with *Mobile Reagents*

Yield101

- Prepares a printable PDF summary of the reaction

- Takes a hard copy to the lab...

- ... performs the experiment. Enters the yield data, shares the scheme with *MolSync*.

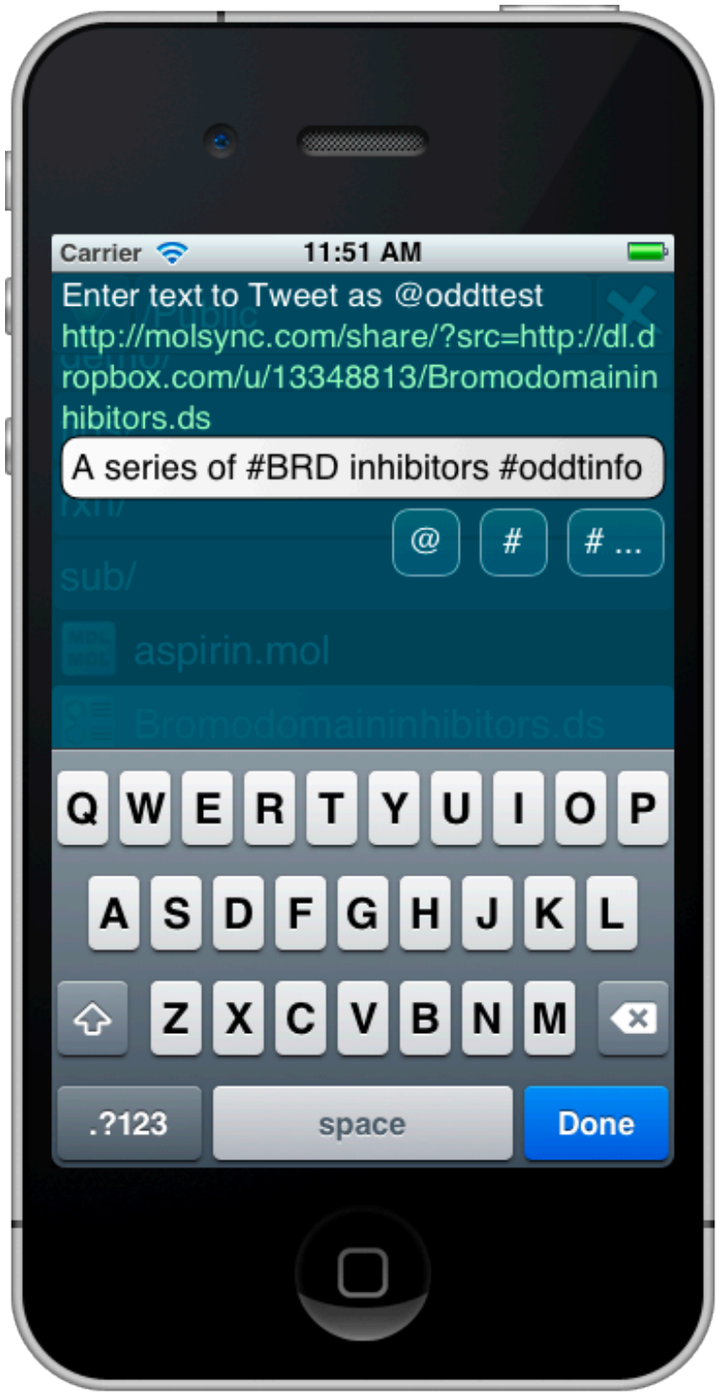


MolSync

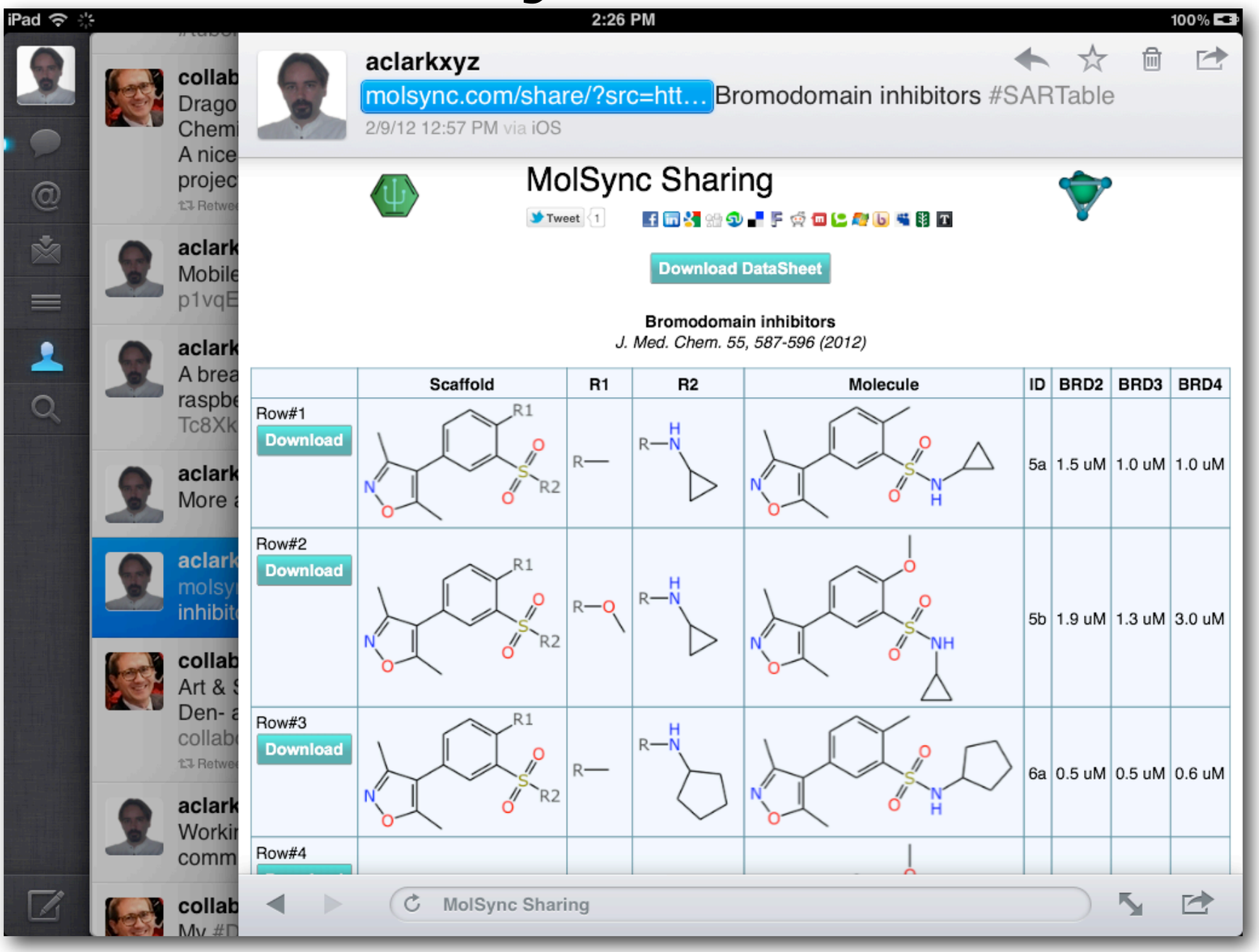
- A number of chemical data files have been created and shared on a *Dropbox* account

- Files in the **Public** folder can be shared on the web, or tweeted

- Tweeting certain hash tags has interesting effects



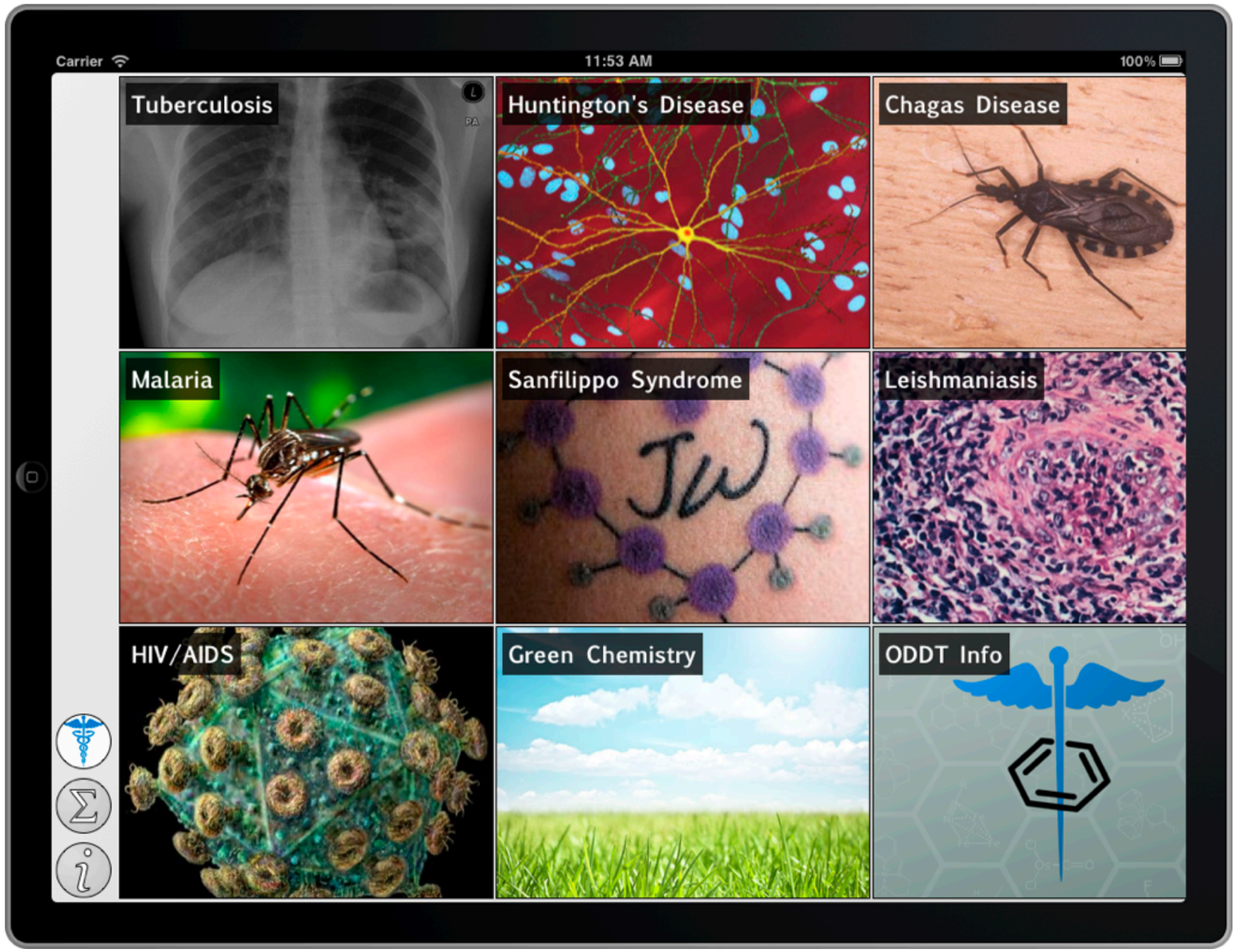
MolSync web



- Raw presentable data wrapped by HTML5 layer: can view, download, render, convert...

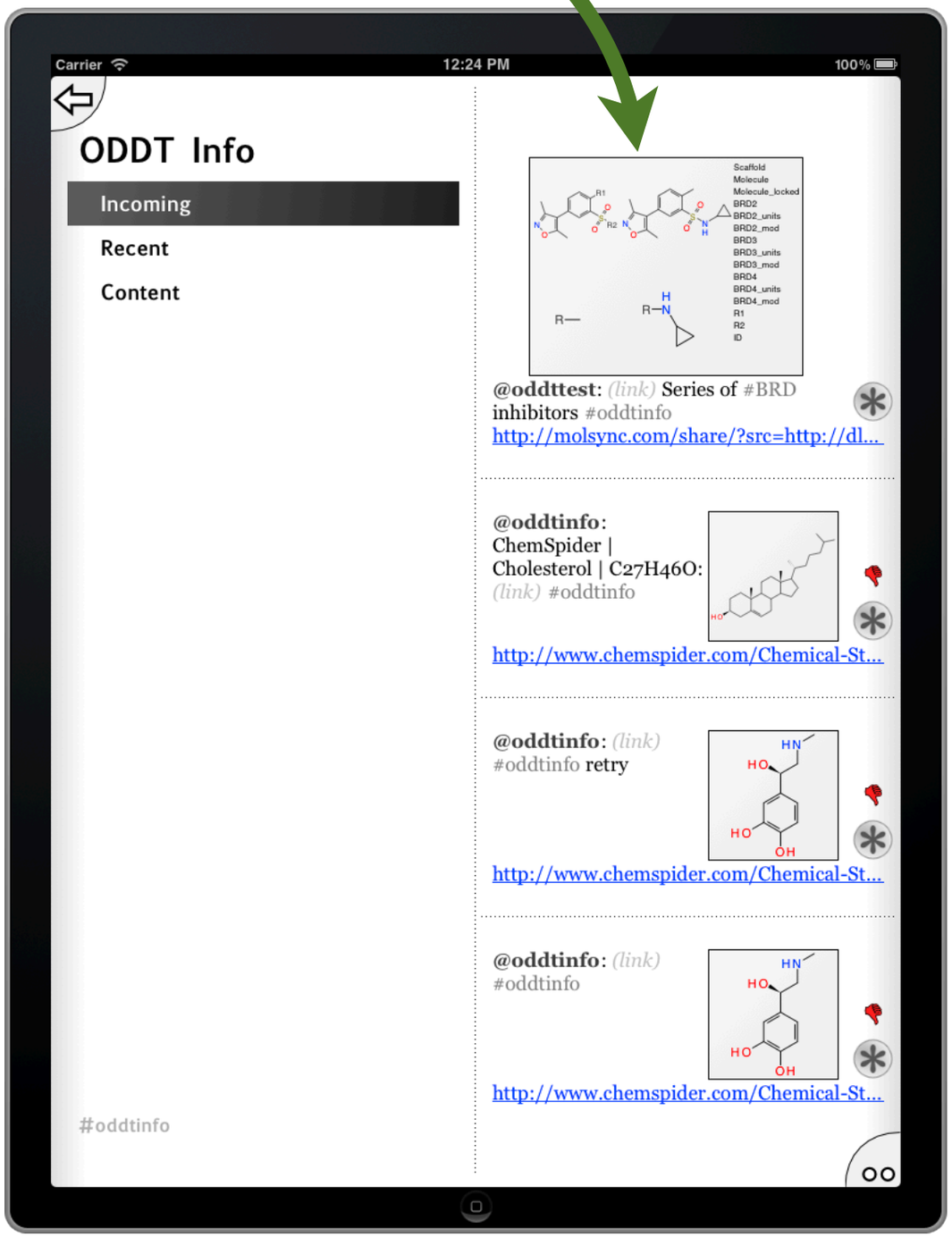
Open Drug Discovery Teams (ODDT)

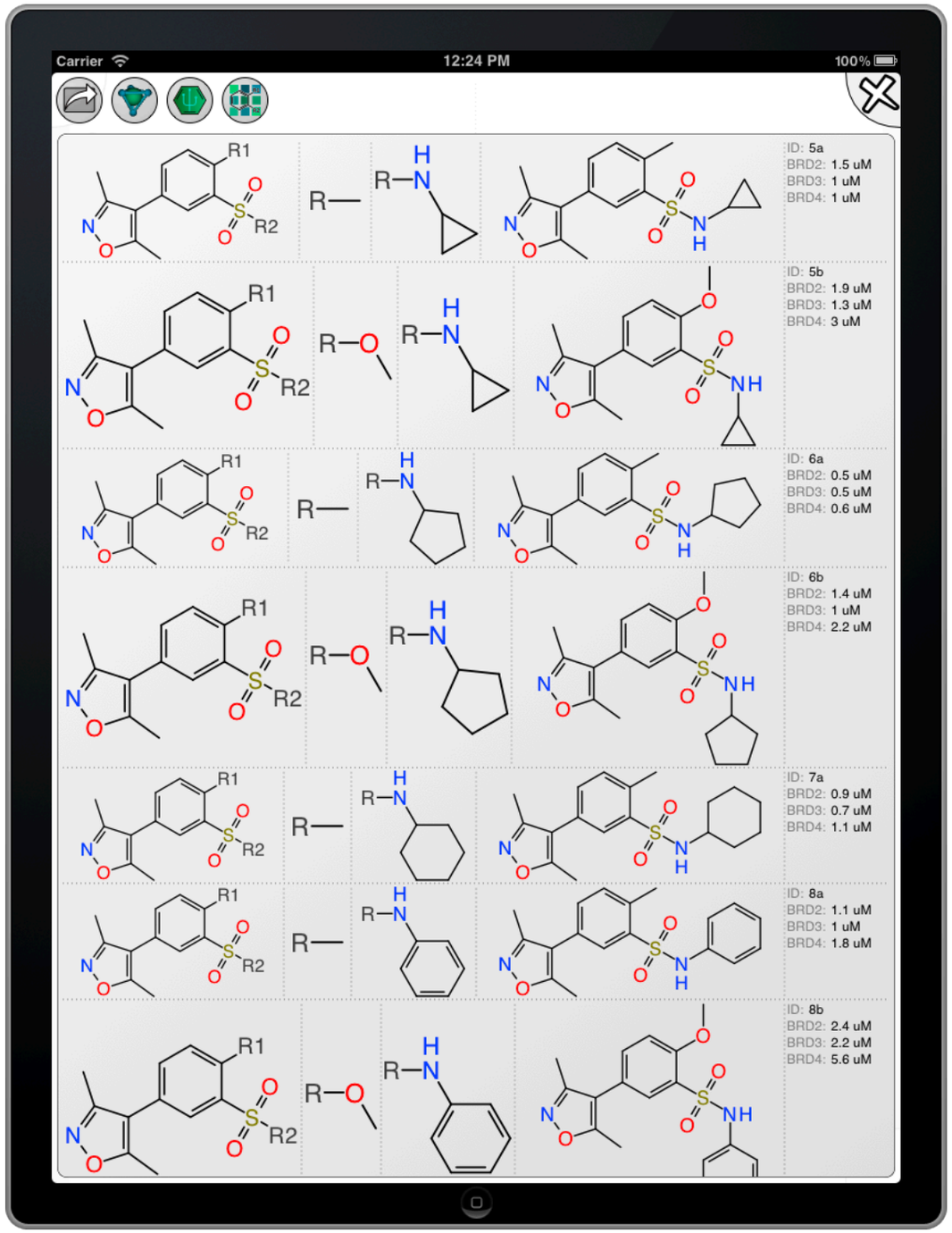
- Aggregates open data from Twitter
- Crowd-sourced curation
- Flipboard-like app interface
- Free. Current alpha testing



from MolSync

ODDT





Acknowledgments

Steve Muskal, **Maurizio Bronzetti**

Eidogen-Sertanty

Peter Löw, **Josef Eiblmaier**, and others

InfoChem

Antony Williams

Royal Society of Chemistry

Sean Ekins

Collaborations in Chemistry

http://molmatinf.com
http://molsync.com
http://cheminf20.org

@aclarkxyz