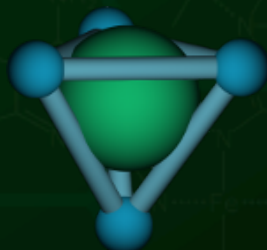


Mobile chemistry apps participating in the open science revolution

Dr. Alex M. Clark

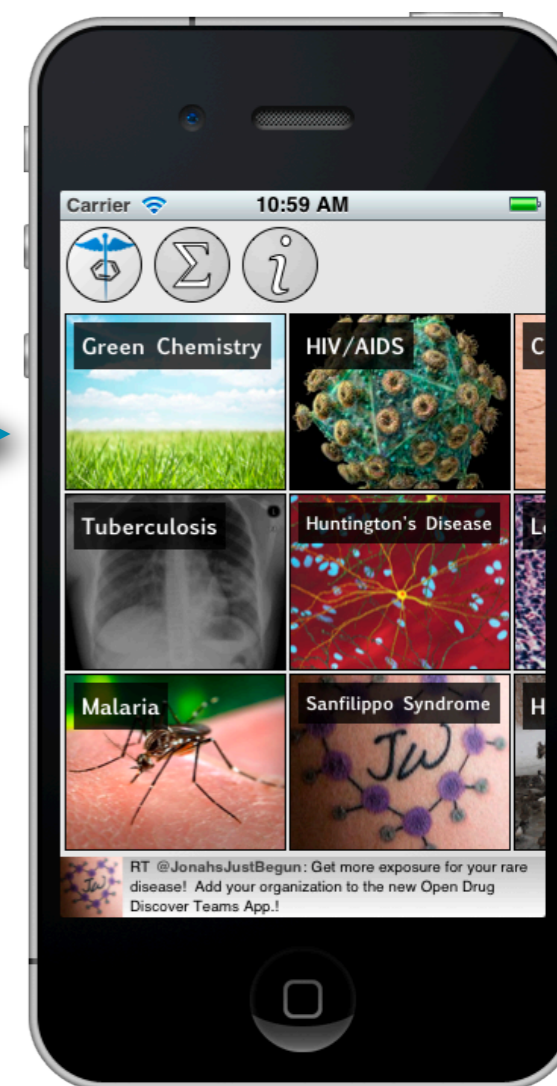
August 2012



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<http://molmatinf.com>

Chemical data



Content creation:
rate limiting step on
mobile devices

Content consumption:
gets interesting with
structured data

Content creation

- Mobile apps hit the ground running with content consumption
- Creation has moved at variable rates depending on industry
- Chemistry late to the party: drawing structures on a cellphone is rather tricky!

Structure Drawing

- Now quite a few options
- Most of them inherit the "ChemDraw style", which is in turn based on 1980s painting tools
- Some are adequate for simple tasks on a tablet, but for a phone, fingers are just too big



Gestures & Templates

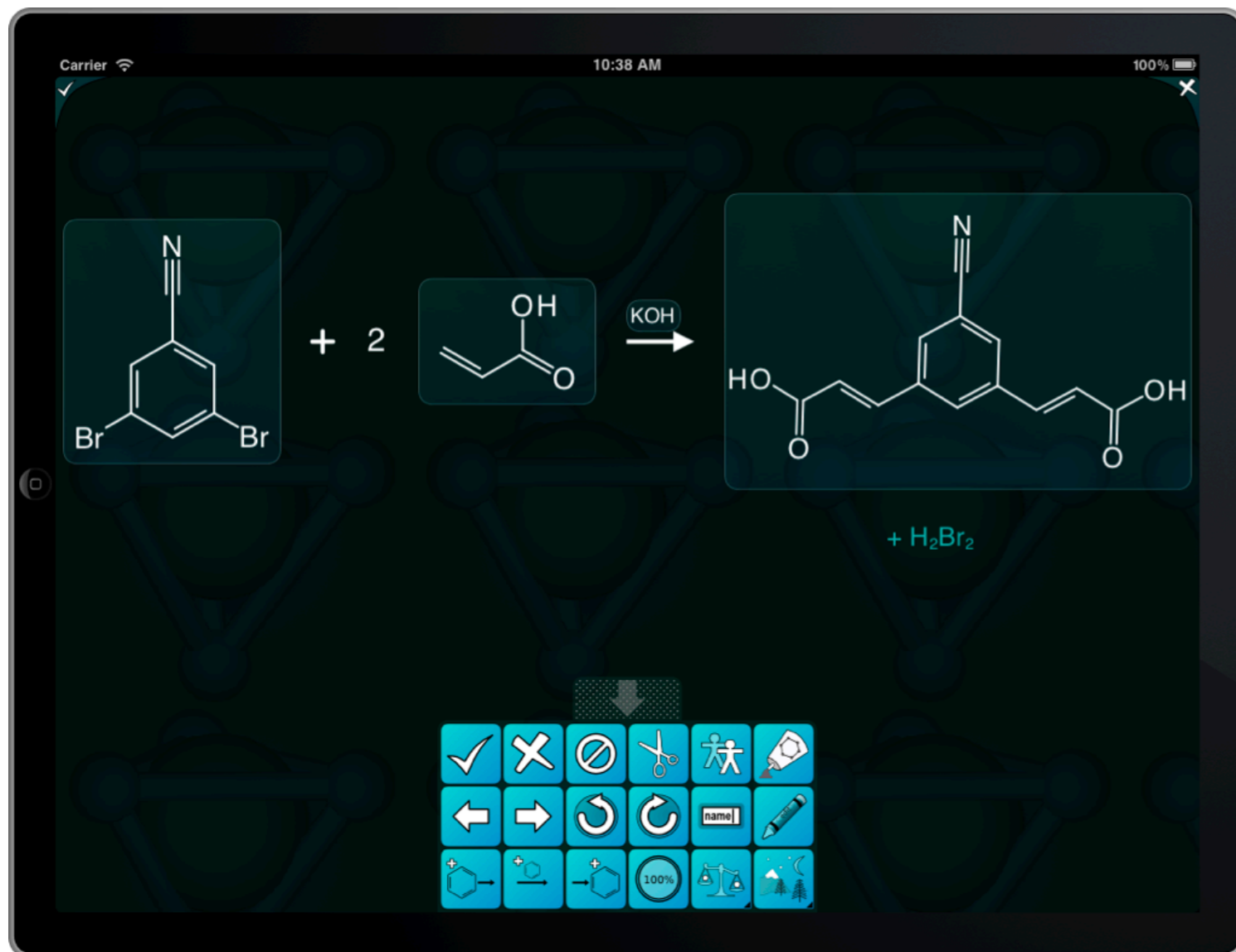
- 2010 introduced the **Mobile Molecular DataSheet** (MMDS) app: can draw publication quality structures quickly on any form factor

Journal of Cheminformatics, **2:8** (2010)

- **Power, speed, simplicity**: pick two
- Now multiple options, to ease the learning curve, or eliminate it

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

Reactions



- Built-in reaction component editor:
 - reactants
 - reagents
 - products
- Handles stoichiometry and reaction balancing

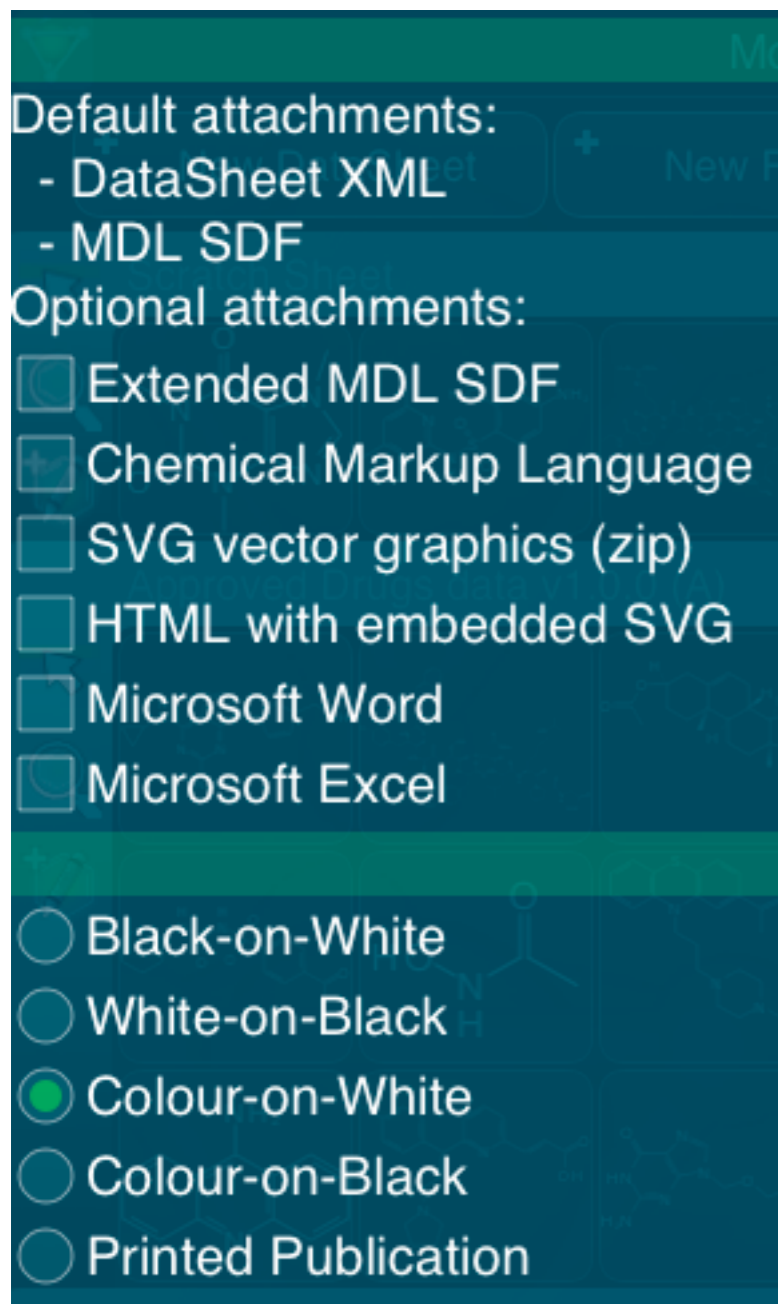
- Separating components is better for lab notebook style: data is more highly structured

DataSheets



- Can create and manage datasheets of molecules, reactions, numbers, text...
- A datasheet can be manipulated as an object: e.g. shared, imported, exported, etc.

Sending data out



- Many formats:

- MDL: **MOL, SDF, RDF, RXN**

- **CML**

- **SMILES, CurlySMILES**

- Bitmap: **PNG**

- Vector: **SVG, EPS, HTML**

- Office: **DocX, XlsX**

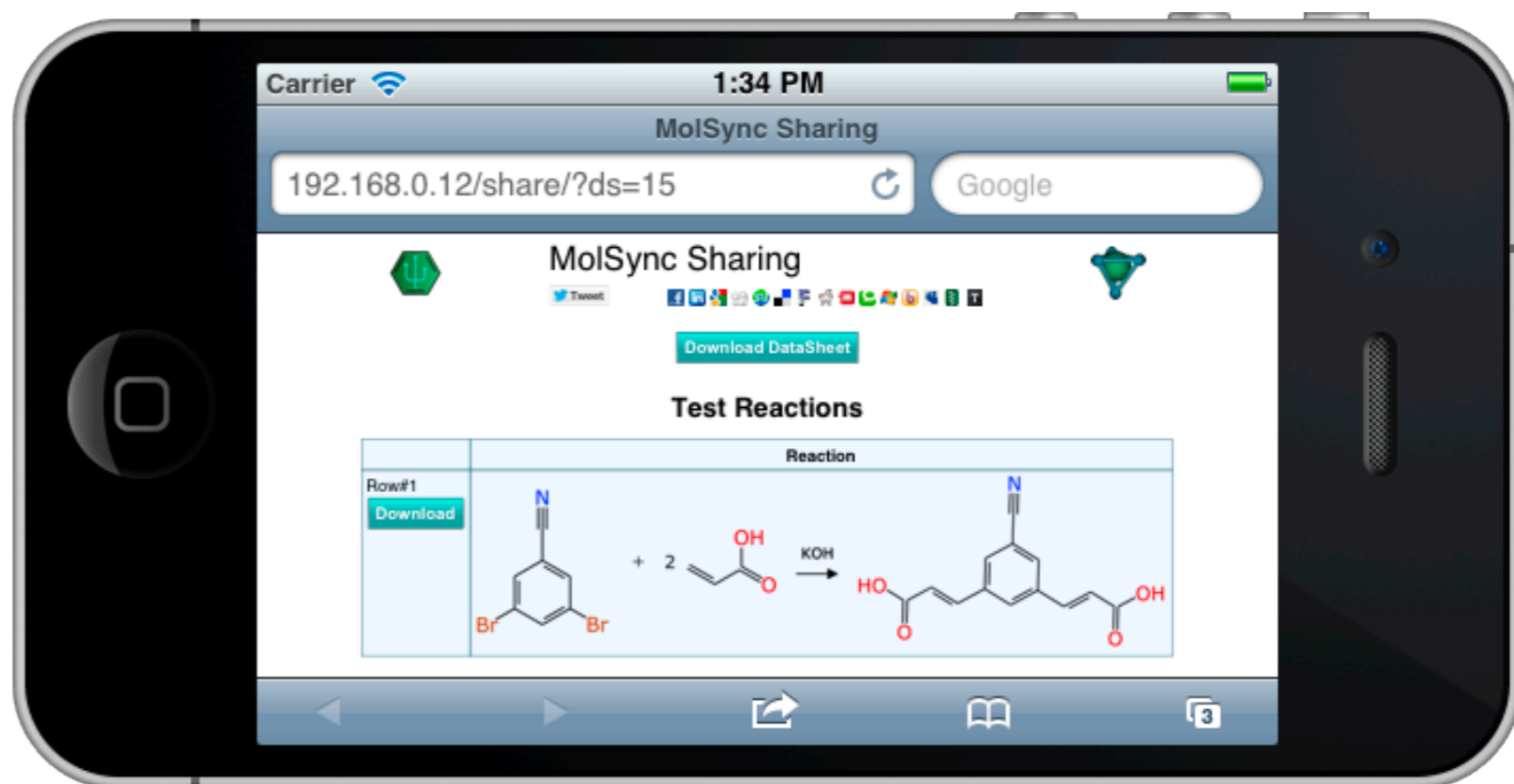
- Zip: *multiple files*

- Some of the output formats require webservice support

Sharing on the Web



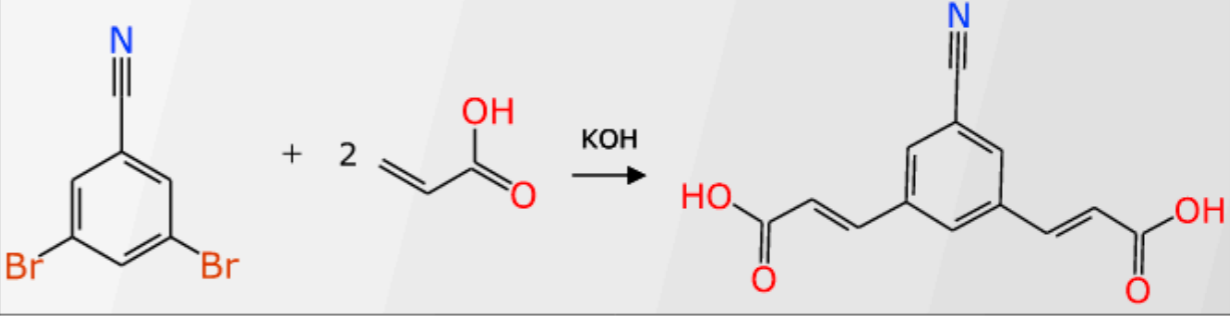
- Can upload molecule, reaction or datasheet to **molsync.com**
- A link is generated: can access with any browser, mobile or otherwise



Web viewing

- The link is *not just a static image*
- **molsync.com** stores the chemical data and renders it as necessary
- The web app allows dynamic
 - format conversion
 - graphics creation
 - property calculation

Download DataSheet ✕



Choose Format

- DataSheet XML
- MDL RDF (reactions + data)
- MDL RXN (single reaction)
- PNG image (raster)
- SVG picture (vector)
- Encapsulated PostScript (vector)
- ZIP (multiple PNG files)
- ZIP (multiple SVG files)
- HTML with embedded SVG
- Microsoft Word
- Microsoft Excel

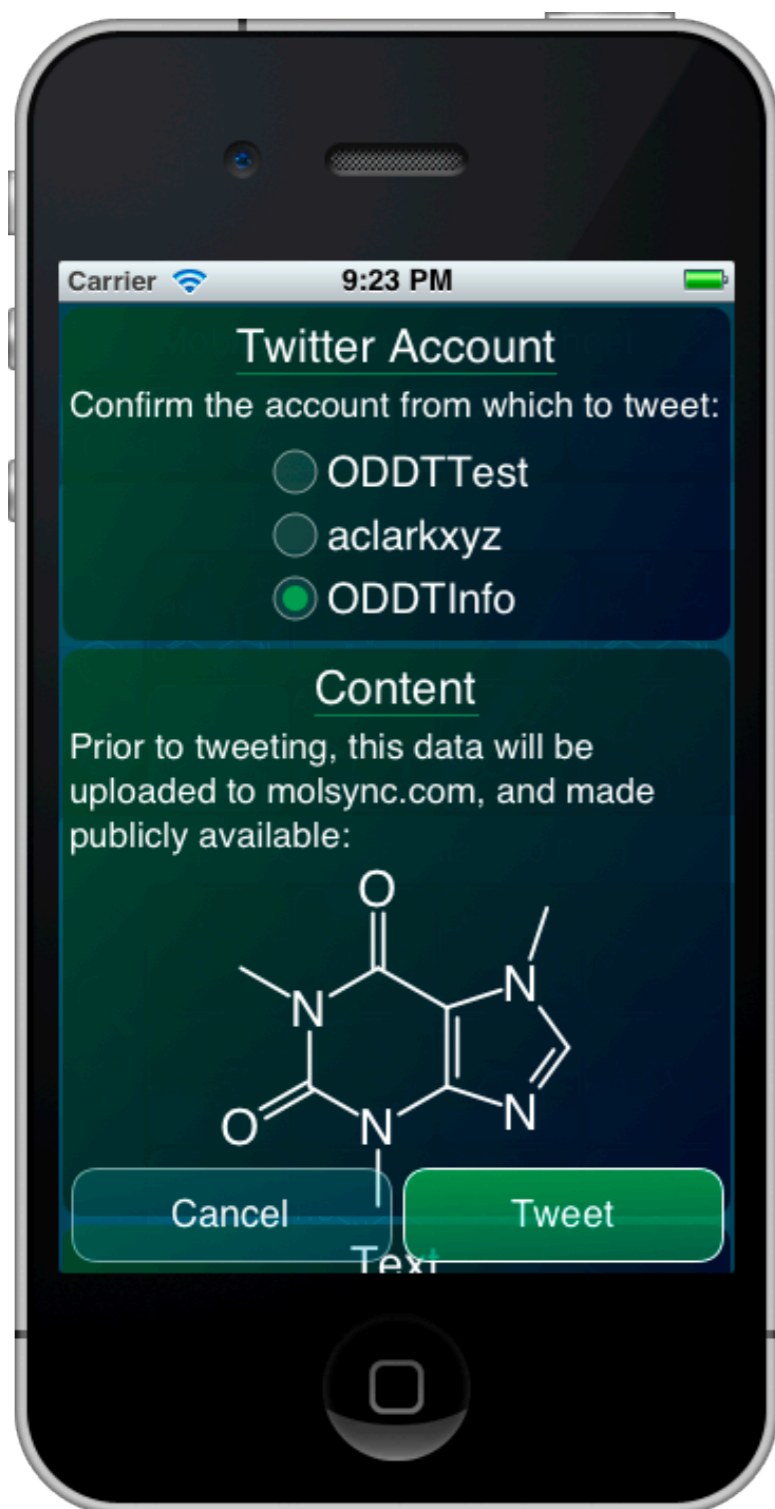
Graphic Options

Sizing: Scale Box

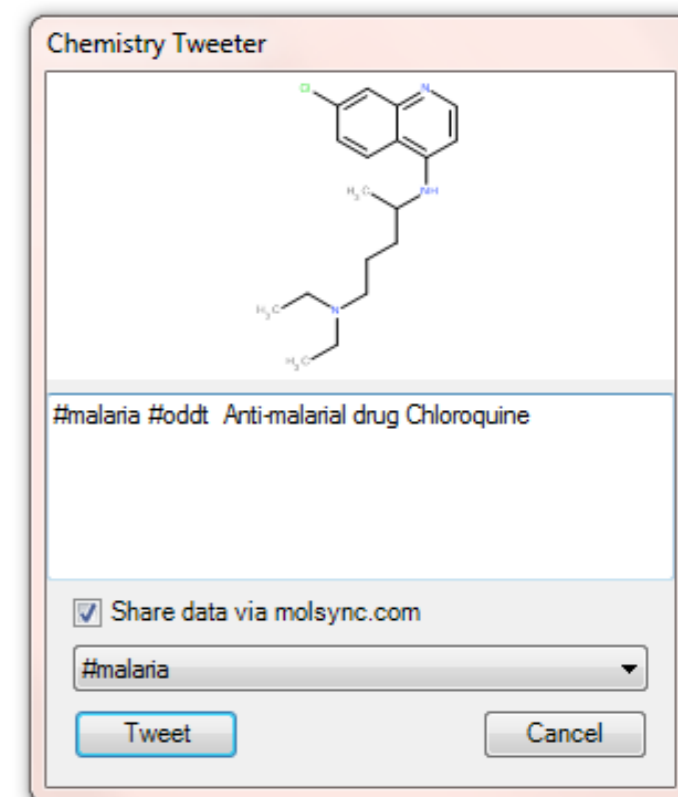
Angstroms-to-Points:

Rendering:

Tweeting



- Several apps allow in-app tweeting of molecules, reactions and datasheets
- As for web sharing: data is uploaded to **molsync.com**
- Tweet contains link for viewing & using
- Can also use [James Jack's Accelrys Draw](#) plugin



Watch the hashtags

The screenshot shows an iPad interface with a tweet from user 'aclarkxyz' posted on 2012-06-20 at 12:41 PM. The tweet contains a link to 'molsync.com/share?ds=18' and two hashtags: '#drugrepurposing' and '#ODDT'. The tweet content is a MolSync Sharing page for 'Approved Drugs data v1.0.0 (B)'. The page features a table with two rows of drug data, each with a 'Download' button and a chemical structure.

	Data	Depicted
Row#1	<p>Name: bacampicillin CSID: 390135</p>	
Row#2	<p>Name: bacitracin CSID: 10481985</p>	

certain tags have special meaning...

Content aggregation

#malaria

#tuberculosis

#huntingtons

#hivaids

#sanfilipposyndrome

#chagas

#greenchemistry

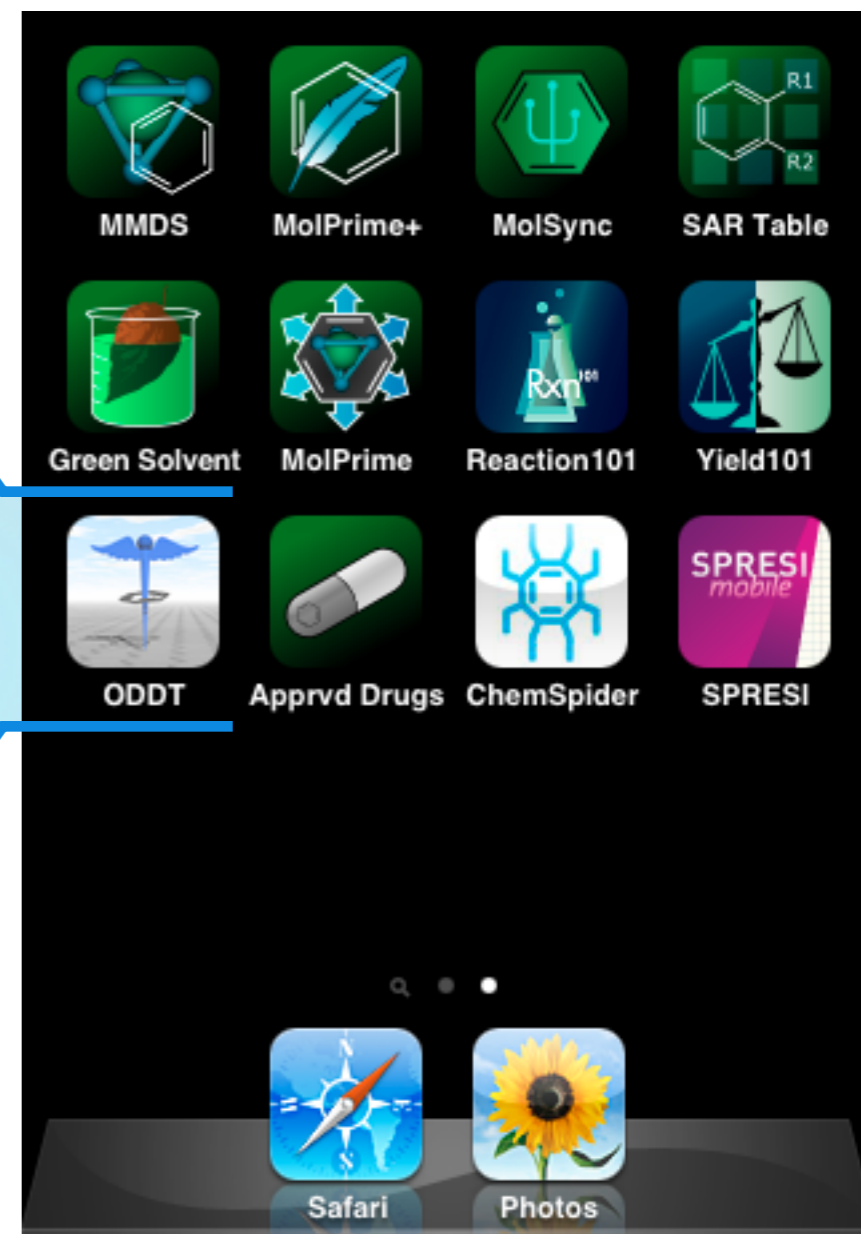
#huntersyndrome

#leishmaniasis

#drugrepurposing

#H5N1

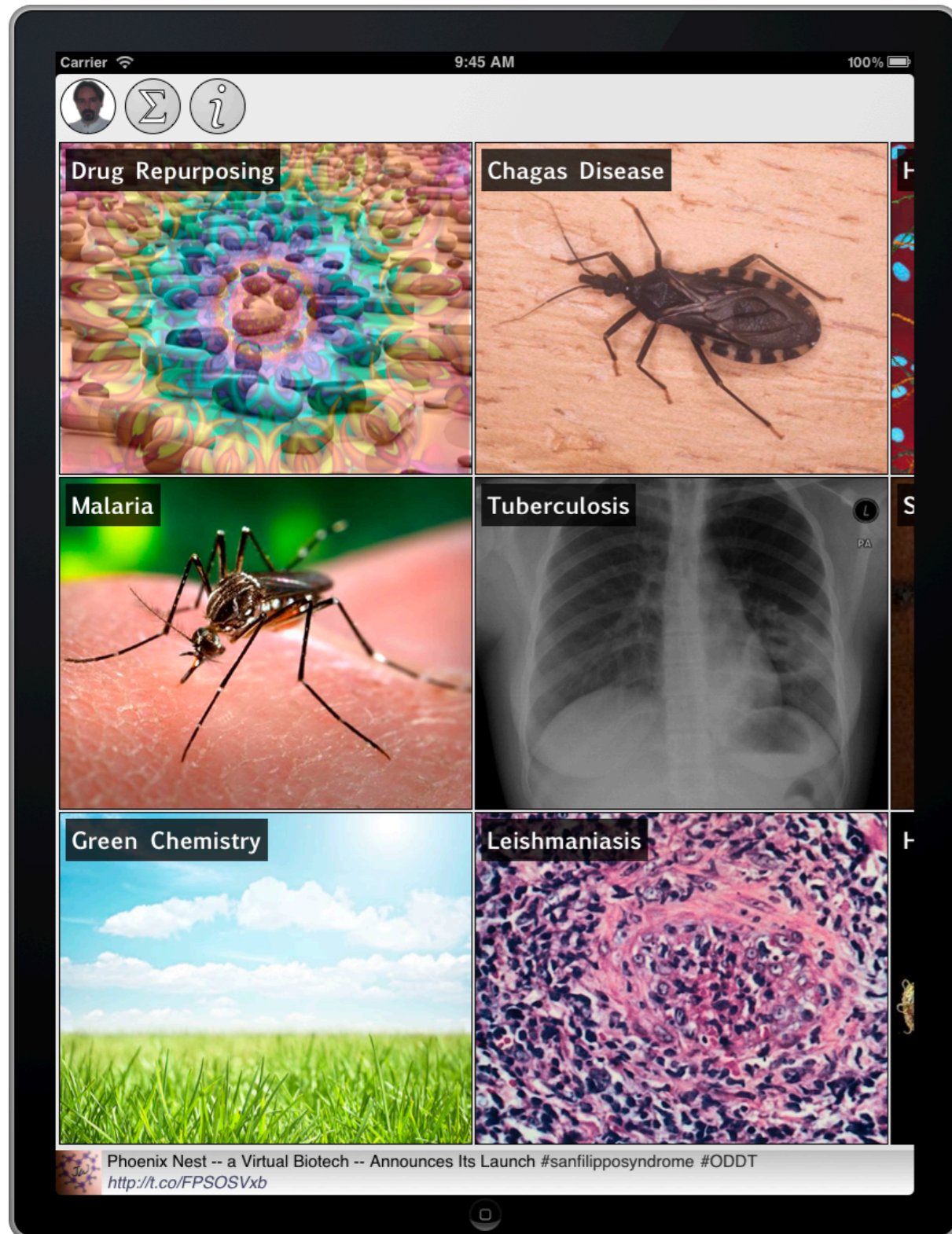
#hhf5gan



<http://bit.ly/Rdn890>

Open Drug Discovery Teams

with Sean Ekins, Collaborations in Chemistry



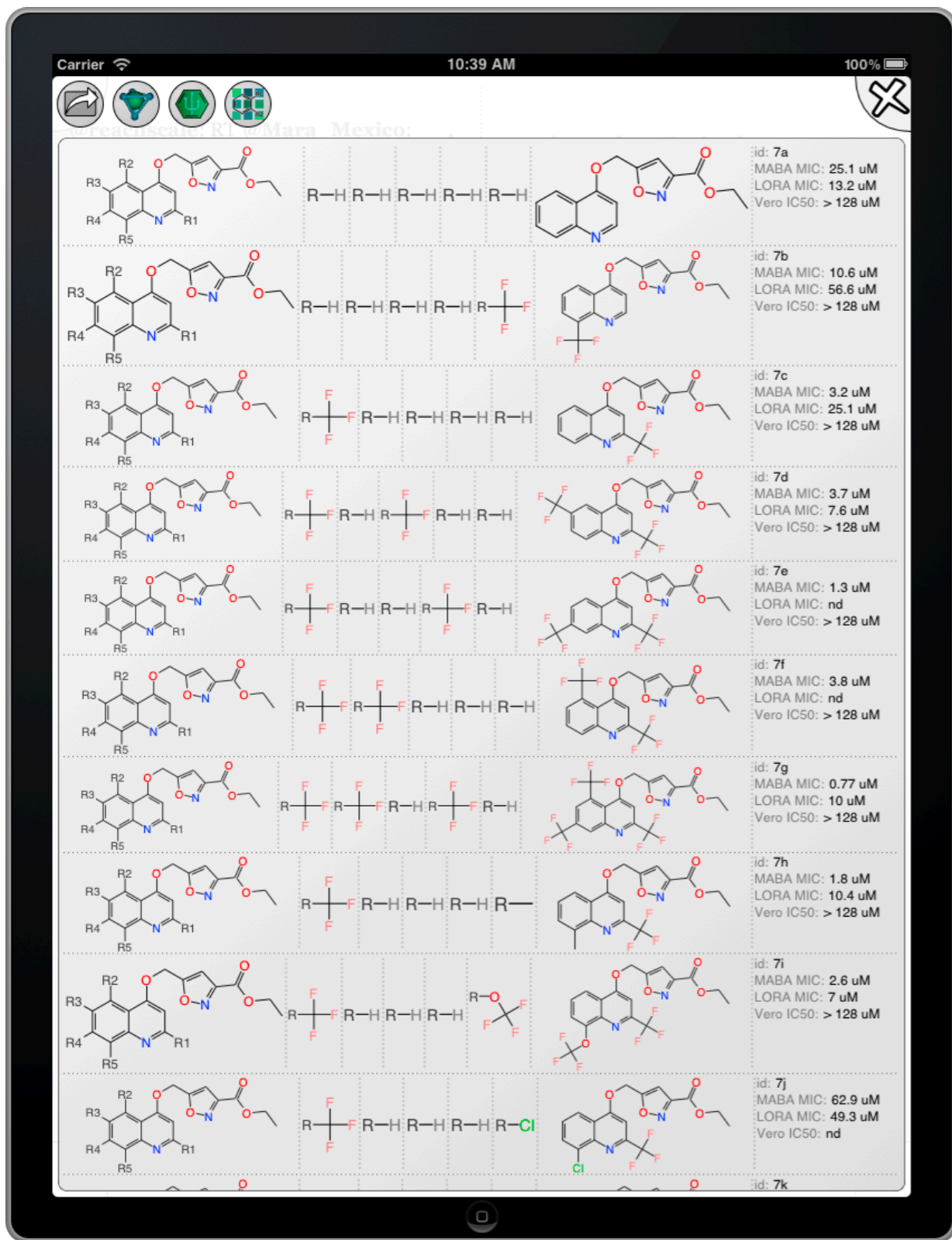
- Server harvests tweets and RSS feeds into topics
- Interface provided via a free app
- All data is open
- Most topics are precompetitive or open-friendly: many rare & neglected diseases

Topic browsing

The screenshot shows a mobile application interface for 'Drug Repurposing'. At the top, there is a status bar with 'Carrier', signal strength, '10:06 AM', and '100%' battery. Below the status bar is a navigation bar with a back arrow and the title 'Drug Repurposing'. A sidebar menu on the left contains 'Incoming', 'Recent' (highlighted), 'Content', and 'Sponsors'. The main content area features a header 'Drug Repurposing Projects :: Department of Internal Medicine | The' with a green heart icon and a star icon. Below this is a row of three chemical structures with a blue arrow pointing from the first to the second. A URL <http://medicine.unm.edu/informatics/pr...> is displayed below. The next section shows a grid of chemical structures with a table header: 'Molecule Name', 'Formula', 'FW', and 'Molecule Name'. Below the grid is a tweet from '@collabchem' with the text '#drugrepurposing #ODDT Compounds identified in Vitro with new activities Pharm Res 28:1785-91 (2011)' and a URL <http://molsync.com/share/?ds=22>. The final section shows another grid of chemical structures with a table header: 'Molecule Name', 'Formula', 'FW', 'Product name', and 'Info'. Below this is another tweet from '@collabchem' with the text '#drugrepurposing #ODDT Orphan-designated products with at least one marketing approval for a common disease indication' and a URL <http://molsync.com/share/?ds=21>. At the bottom left, the hashtag '#drugrepurposing' is visible. The bottom right corner has a double-circle icon.

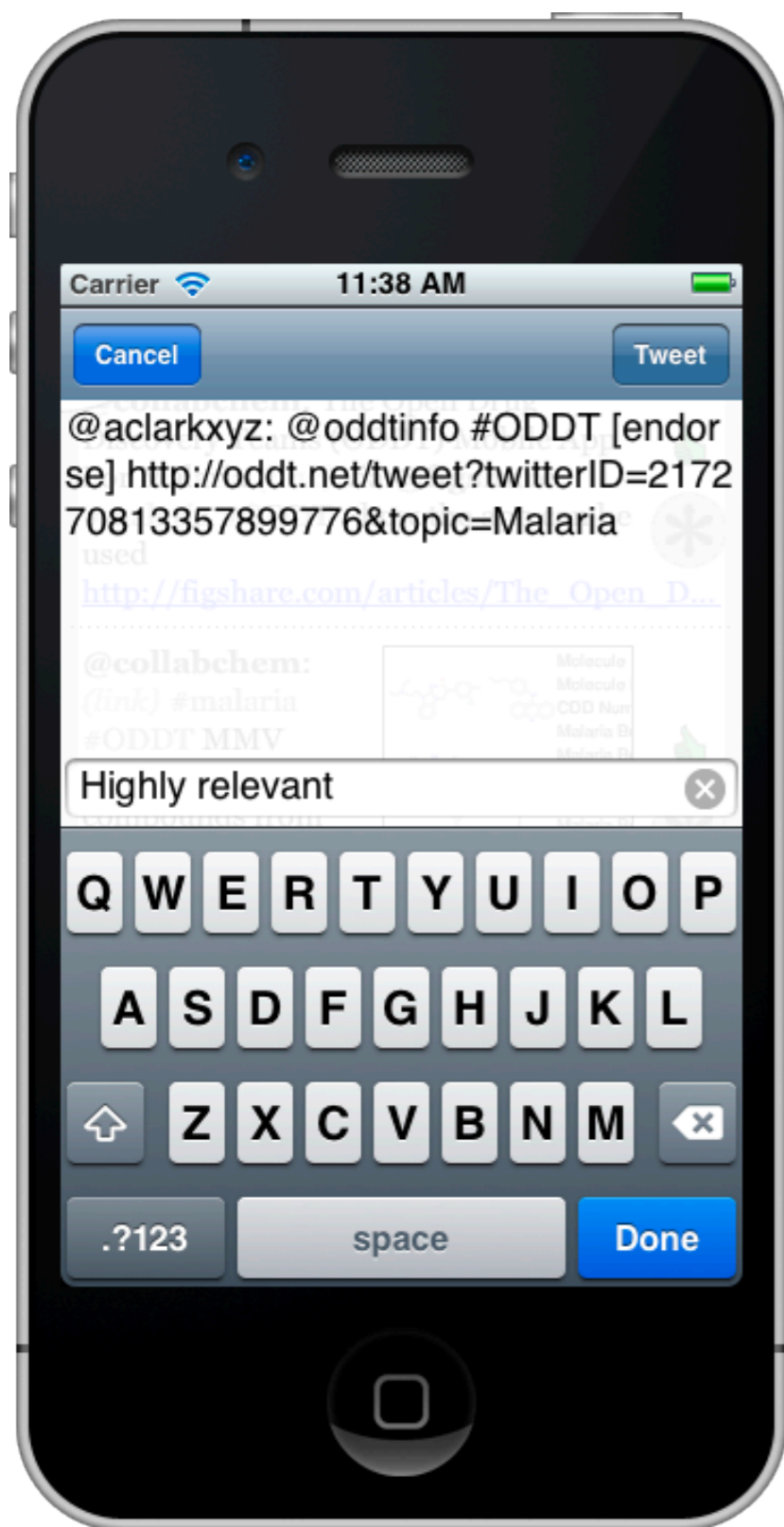
- Browse article headings and thumbnails
- Tap to view
 - links
 - images
 - chemical data

Chemical awareness



- App & server both understand chemical data
- Inline viewing of molecules, reactions, datasheets, SAR tables
- Can use *open with* to send the data to other apps... e.g. **MMDS**, **MolSync**, **SAR Table** ...

Crowd curation



- Emit tweets from within the app to affect content
- Can **endorse** or **disapprove**: votes content up or down
- Anything that fails to achieve +ve endorsement eventually deleted
- Many more annotation modifiers planned

Plans

- Add more **open friendly** topics, e.g. rare & neglected diseases
- To add **cheminformatics** features to the back end, e.g. structure searching, activity compilation, SAR table generation...
- More integration with other apps, to make it useful as a real time **lab notebook**
- Extend the **crowd sourcing** features: evolve it into a micropublishing platform

Conclusion

- Opportunities abound for mobile apps to participate in open science
- Much of the technology already exists
- Tweet your papers and your data, with hashtags
- Get involved, find out what is missing, and get in touch!

<http://molmatinf.com>

<http://molsync.com>

<http://cheminf20.org>

@aclarkxyz

