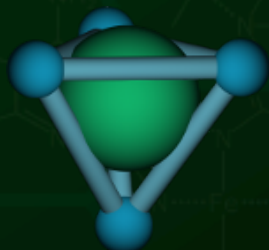


# Open Drug Discovery Teams

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

**Dr. Alex M. Clark**  
**Dr. Sean Ekins**

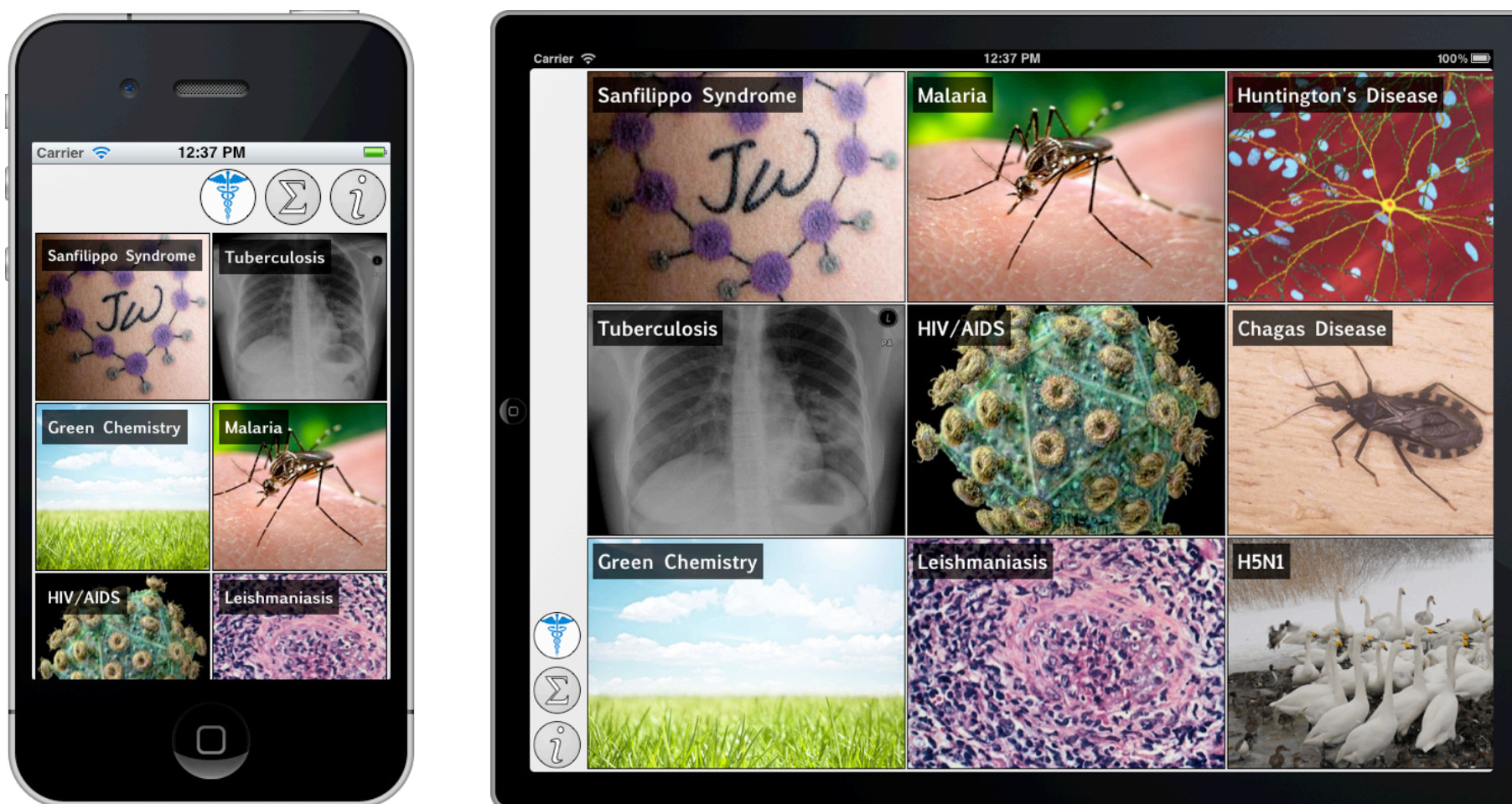
June 2012



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and Collaborations in Chemistry

# App Overview

- Content aggregator for open chemistry topics such as rare and neglected diseases
- Multiple collection sources, crowd-curated evaluation



- Open data, free mobile app for iPhone, iPod, iPad



# Availability

- Open Drug Discovery Teams (ODDT) is available **free** from the Apple iTunes AppStore



<http://itunes.apple.com/app/oddt/id517000016>

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

# Features

- Magazine-like interface to medicinal chemistry topics, e.g. rare & neglected diseases
- Data gathered from *Twitter* hashtags and RSS feeds
- Inline browsing of web documents
- Intelligent handling of chemical data (e.g. molecules, reactions, auxiliary data)
- Crowd-curation: endorse, disapprove or comment by emitting a *tweet*



# Topics

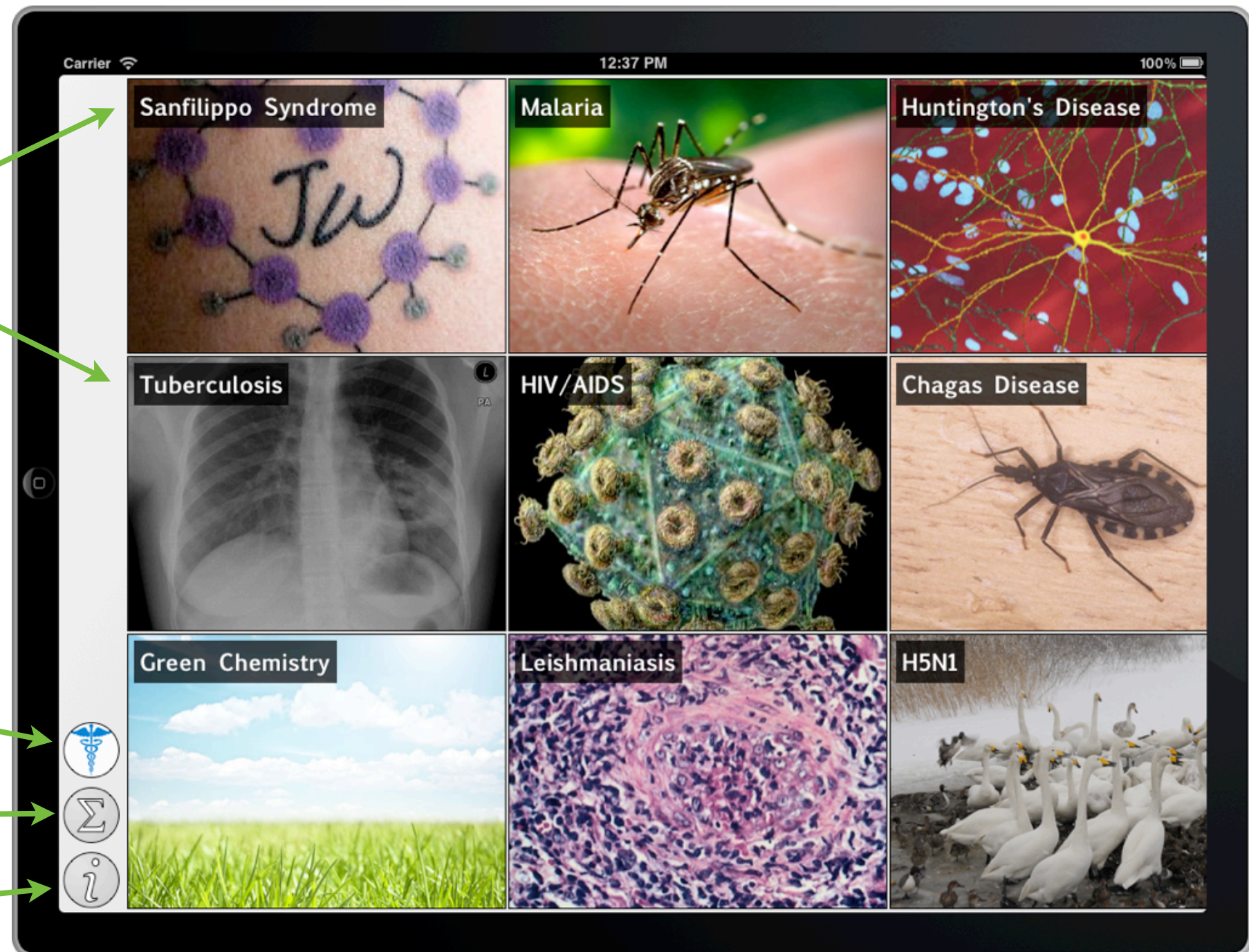
- Current topics focus on rare & neglected diseases, and other precompetitive areas such as green chemistry and drug repurposing

Each panel represents a topic

Twitter user

User stats

About info



# Browsing

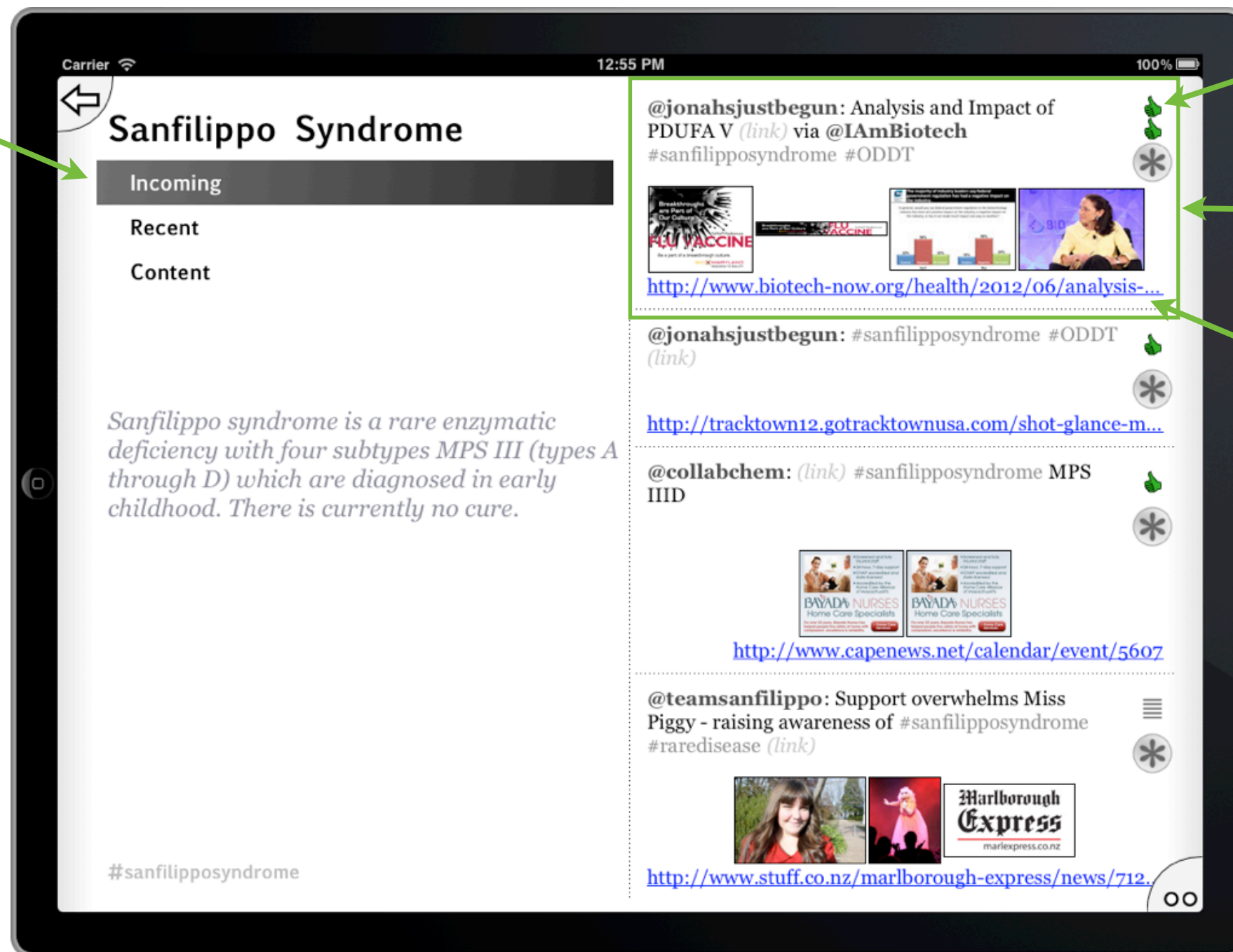
- Entries are displayed in pages, most recent first

Filters

Endorsements

Entry

Viewable  
link



# Crowdsourcing

- Anyone can tweet data with topic hashtags, e.g. #malaria, #sanfilipposyndrome, #greenchemistry
- Links will be harvested and added to the collection
- Can adjust existing content:

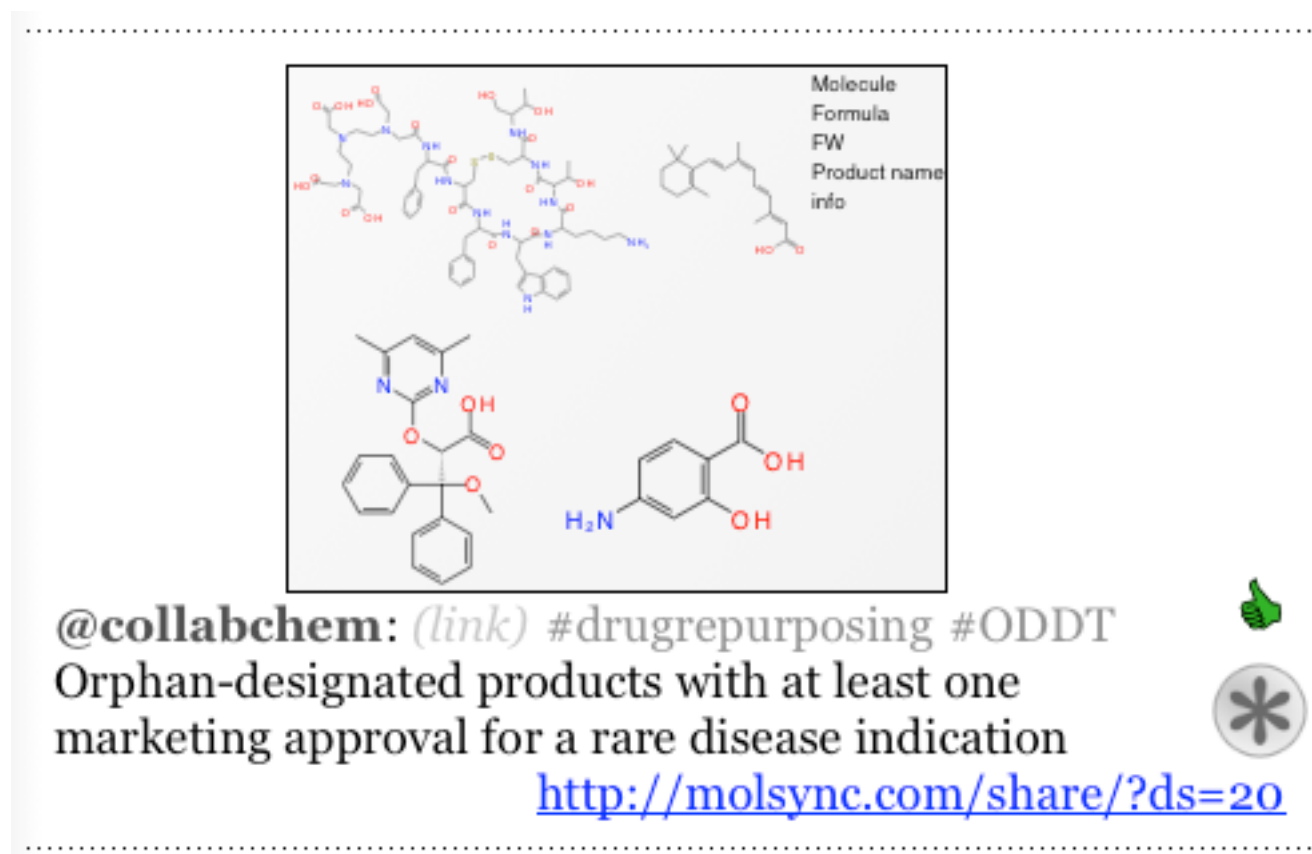


- Emits a tweet from within the app, which affects the



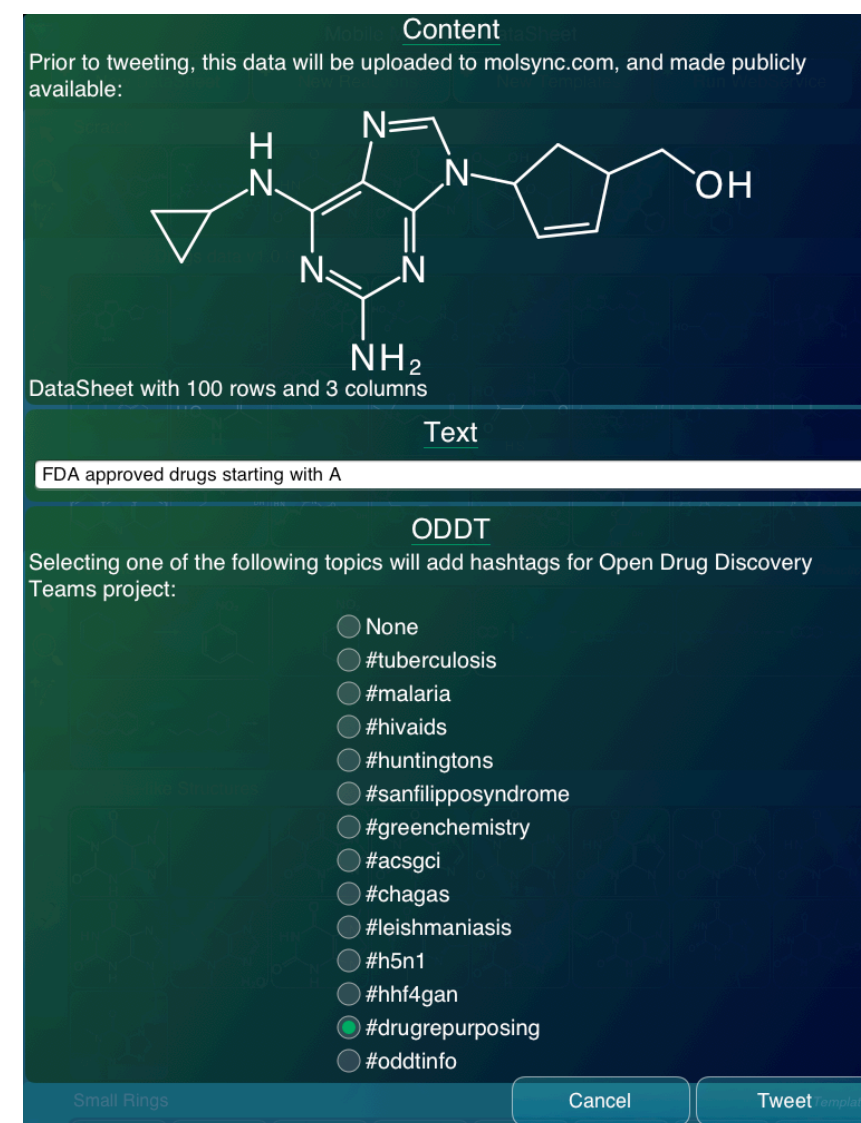
# Chemistry

- ODDT understands links chemical data, and has special viewing, manipulation and collaboration features for molecules and reactions



The screenshot shows a tweet interface. At the top, there's a box containing several chemical structures. To the right of these structures is a table with the following headers: Molecule, Formula, FW, Product name, and info. Below the structures, the tweet text reads: "@collabchem: (link) #drugrepurposing #ODDT Orphan-designated products with at least one marketing approval for a rare disease indication". Below the text is a blue link: <http://molsync.com/share/?ds=20>. To the right of the text and link are icons for liking (a thumbs up) and retweeting (a star).

- Other apps such as the Mobile Molecular DataSheet allow direct tweeting of chemical data with ODDT topic hash tags...



The screenshot shows the Mobile Molecular DataSheet app interface for tweeting. At the top, it says "Content" and "Prior to tweeting, this data will be uploaded to molsync.com, and made publicly available:". Below this is a chemical structure of a molecule. Underneath the structure, it says "DataSheet with 100 rows and 3 columns". Below that is a "Text" field containing "FDA approved drugs starting with A". At the bottom, there's a section titled "ODDT" with the text "Selecting one of the following topics will add hashtags for Open Drug Discovery Teams project:". Below this is a list of topics with radio buttons: None, #tuberculosis, #malaria, #hiv, #hiv, #huntingtons, #sanfilipposyndrome, #greenchemistry, #acsgci, #chagas, #leishmaniasis, #h5n1, #h5n1, #h5n1, #drugrepurposing (which is selected), and #oddinfo. At the bottom right are "Cancel" and "Tweet" buttons.



# Future Developments

- The Open Drug Discovery Teams project is currently a minimum viable product
- New developments are happening fast, e.g.
  - More topics
  - New data sources
  - Advanced cheminformatics
- Your feedback is welcome. Download the app, try it out, and get in touch!

# In the literature

- A.J. Williams, S. Ekins, A.M. Clark, J. Jack, R. Apodaca, "Mobile apps for chemistry in the world of drug discovery", *Drug Discovery Today*, **16**, 928-939 (2011)
- A.M. Clark, A.J. Williams, S. Ekins, "Redefining Cheminformatics with Intuitive Collaborative Mobile Apps", *Molecular Informatics*, manuscript in press.
- S. Ekins, A.M. Clark, A.J. Williams, "Open Drug Discovery Teams: A Chemistry Mobile App for Collaboration", *Molecular Informatics*, manuscript in press.

# More Information

<http://oddt.net>

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

<http://cheminf20.org>

<http://collabchem.com>

**@aclarkxyz**  
**@collabchem**

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