

Open Drug Discovery Teams

(ODDT)

USER GUIDE and FAQs– Beta version

v0.90

April 2012

Dr. Sean Ekins

Collaborations in Chemistry, A division of Collaborations in Communications, Inc.

Dr. Alex M. Clark

Molecular Materials Informatics, Inc.

Project Description

The Open Drug Discovery Teams (ODDT) project provides a mobile app primarily intended as a research topic aggregator of open science data integrated from various sources on the internet.

User Guide

The entry screen to the app displays the topics ranked by use (Fig. 1). Tapping a topic image opens the topic browser, starting with the *incoming* page. Newly added content is listed on the right (Fig. 2). Each tweet that has been introduced into the data collection is referred to a *factoid*. A factoid can be endorsed or disapproved (Fig. 3), and the hyperlinks can be followed. The *recent* page shows factoids with one or more vote (Fig. 4) while the *content* section shows the most popular voted content in rank order (Fig. 5). Molecule thumbnails can be tapped to open in other apps like *MolSync* (Fig. 6A) or *SAR Table* (Fig 6B). Back on the entry screen, tapping the statistics summary button opens a listing of endorsements, disapprovals, injections and retirements for each hashtag (Fig. 8).

Intended use

We have defined a small number of topics, corresponding to Twitter hashtags such as:

#tuberculosis

#malaria

#hivaids

#huntingtons

#sanfilipposyndrome

#leishmaniasis
#chagas
#h5n1
#greenchemistry

All of these subjects have high potential for positively impacting the research environment using computational approaches and dissemination information via mobile apps.

As the software collection evolves and improves in its capabilities, data from open science will be integrated and made usable within a common framework. Team members will be able to borrow and reuse a growing collection of existing data. Networking and collaboration features will be introduced, allowing researchers to post incomplete or speculative data, while other researchers fill in missing details, and the community as a whole can debate, contest or endorse data based on its quality. ODDT may also contribute to the nascent development of “nanopublications”. The app could also be used as a type of open lab notebook whereby individual researchers share links (URLs) to content and the app aggregates these.

While this system is nominally intended for annotation of content that is fully accessible via the original URL, it is potentially quite useful to annotate documents to which many users do not have access, e.g. articles that are behind a journal pay wall. The collective annotations of the users who have access to the article may provide enough information to allow some users to bypass the purchasing of the article. It also has potential as a path to assemble articles from scratch, in a fully open medium, and institute a kind of informal peer review. In addition this functionality goes further towards an open notebook use case scenario in which the scientist publishes their results whenever a suitable point is reached, whether or not the results are sufficiently complete to warrant dissemination in a traditional peer reviewed article.

FAQ

-What platforms does ODDT run on?

The user interface is provided in the form of an iOS app, which runs on iPhone, iPod and iPad devices. It can be downloaded freely from the Apple iTunes AppStore:

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

Versions for other platforms, such as Android and generic web, are planned, but for the moment we are focusing on the most popular app platform.

-How do I interact with the ODDT app?

When you download and run ODDT, you are able to browse and view any and all of the content, which is free and open. To interact with the system, you must activate your Twitter account. You have to configure Twitter from within the iOS system, and then when the app requests permission to have access, you need to say yes. Once this is done, you can endorse, disapprove or comment on factoids from within the app. This is done by emitting a tweet from your account. The app will never use your Twitter account without making it abundantly clear what is about to happen, i.e. you need to press a button labelled **Tweet**. Once you have connected to Twitter, you will also be able to view the statistics that are associated with your account.

-When I tell my rare disease friends and associates about the app, can I suggest that they offer to add their rare disease?

Later versions of the app will add more disease topics, but by all means get them to send us the disease names to add, along with a suggested Twitter hashtag, and an image to display on the main screen.

-What does the Epsilon icon on the main screen stand for?

This can be used for tracking your activity, based on your Twitter account, both overall and broken down by topic. Each time you endorse or disapprove a factoid, your count goes up. If you tweet out a link to new content, using one of the topic hashtags, and it gets endorsed by you or something else, it counts as an "injection". A "retirement" is a factoid that got deleted due to lack of endorsement, following the one week grace period.

-Where do the topics come from?

The initial choice of diseases/research topics was based on our diverse interests. In future app versions we plan on crowd sourcing the topics, as well as the content and ranking.

-When I tweet something on my account that relates to topicX should I always tag it with: #ODDT #topicX

When you emit a tweet that has a link and one of the topic hashtags, it is assimilated as a factoid. By default it starts with an endorsement rating of 0, which means that it will eventually be retired, unless someone endorses it. If you also add the **#oddt** hash tag, it will auto-endorse, which means that it starts out as a factoid with a +1 ranking, and the endorsement corresponds to the Twitter account you used to post it.

For example:

1. **@researcher**: Progress on a cure for **#malaria** <http://malaria.org/cure.html>
2. **@researcher**: Progress on a cure for **#malaria** <http://malaria.org/cure.html> **#oddt**

The first tweet starts with an endorsement of 0, and will eventually be deleted unless somebody endorses it. The second tweet is equivalent to the first tweet followed by **@researcher** endorsing it.

-Are hashtags case-sensitive?

No. #greenchemistry, #GreenChemistry and #GREENCHEMISTRY are all the same, but #Green_Chemistry is different.

-How do I get my rare/neglected community involved ?

To get your team involved just get them all tweeting the hashtag for the topic of interest. Get the scientists to share links to papers or ideas they want to put out there openly. If we can create a community then we can store the information for mining later and reuse across diseases..e.g. we can tweet molecules, structure activity data, summaries of papers, links to news etc.

Encourage them to download the app, too, but they don't need an iPhone/iPad to participate.

-Whats the difference between Incoming, Recent and Content?

Incoming: all tweets that have been converted into factoids, sorted by latest first. Suitable for browsing for new content worthy of endorsing.

Recent: factoids that currently have a positive ranking, i.e. there is at least one endorsement, and the endorsements are not outweighed by disapprovals. Sorted by time most recently updated.

Content: currently similar to *Recent*, except that highest ranking is shown first.

-What sort of factoids should I endorse?

The ODDT project is about collating open data for research. Factoids that have links to content that resides behind paywalls should probably not be endorsed unless there is a reasonably detailed abstract or synopsis, or if the purpose is to associate links with helpful metadata, e.g. chemical structures, or useful comments. For the disease-related topics, endorsed factoids should have direct or indirect relevance toward finding a cure, such as the ongoing search for a drug, vaccine, antibody, gene-therapy, etc.

-How is the Open Drug Discovery Teams project funded?

Currently it isn't. The beta version was designed and built by Sean Ekins and Alex M.Clark. The server is being temporarily hosted on *molsync.com*. We are interested in exploring a variety of different funding opportunities.

Please contact us for further details at: aclark@molmatinf.com and ekinssean@yahoo.com. You can learn more about the ODDT app at:

http://www.scimobileapps.com/index.php?title=Open_Drug_Discovery_Teams

And frequent blogs at <http://www.collabchem.com> and <http://cheminf20.org>.

Acknowledgments

Photo for tattoo for Jonah's Just Begun (San Fillipo Syndrome) courtesy of Jill Wood
www.jonahsjustbegun.org

Fig. 1.

9 Panels includes one on ODDT information

Can use multiple Twitter accounts user icon

Stats summary

About App

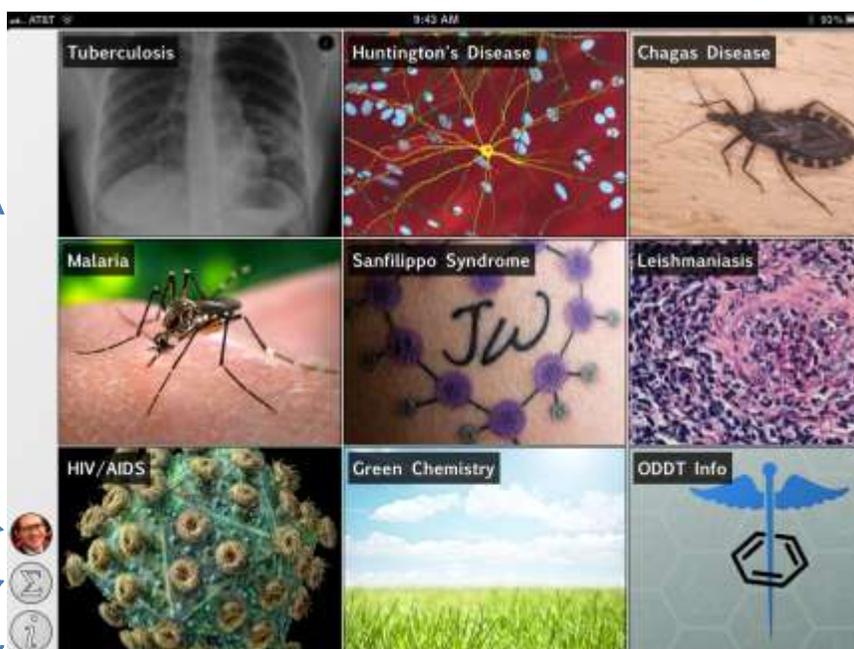


Fig. 2



Click here to endorse or disapprove
Click here to follow hyperlink

Incoming data is sorted by time of creation

Fig. 3

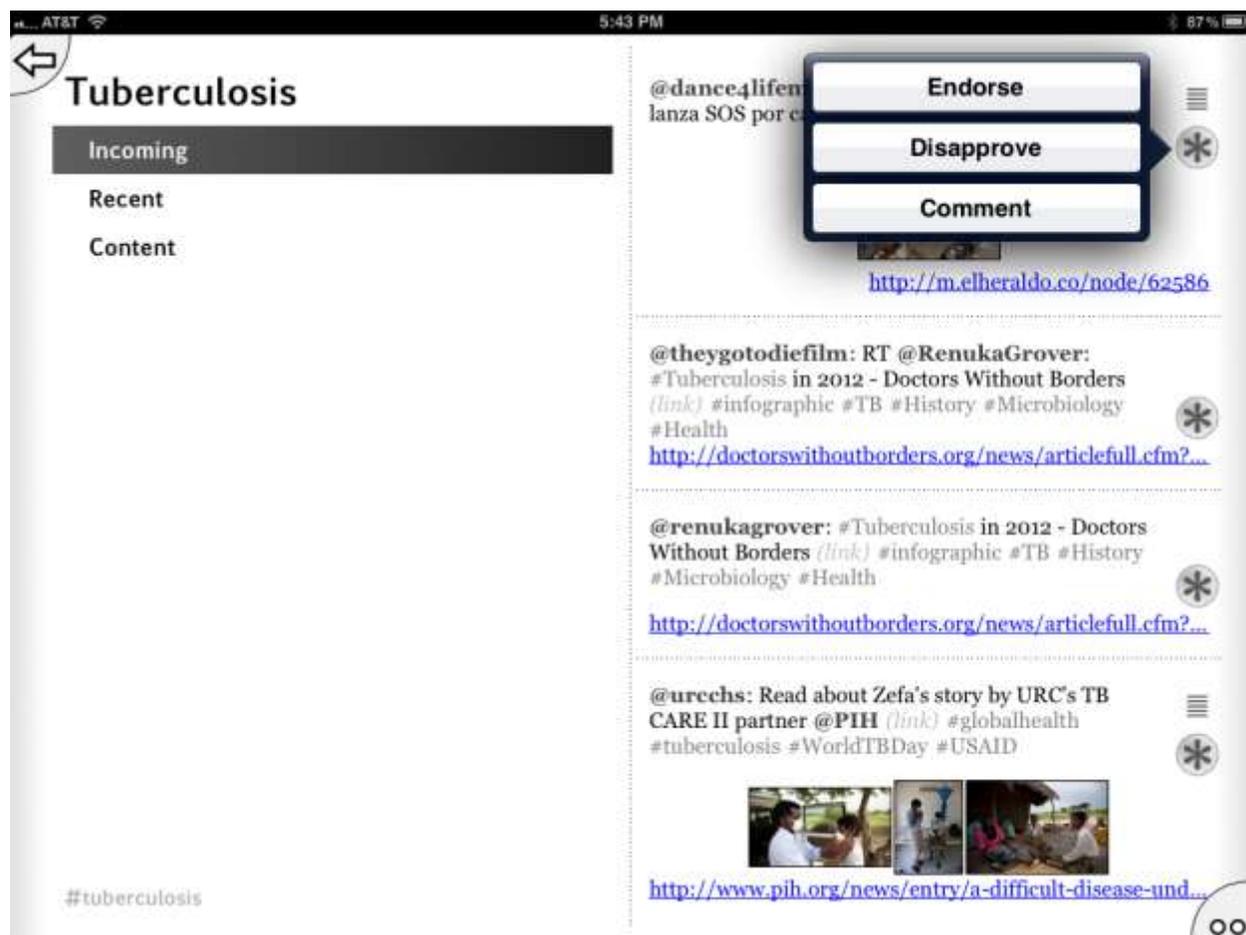
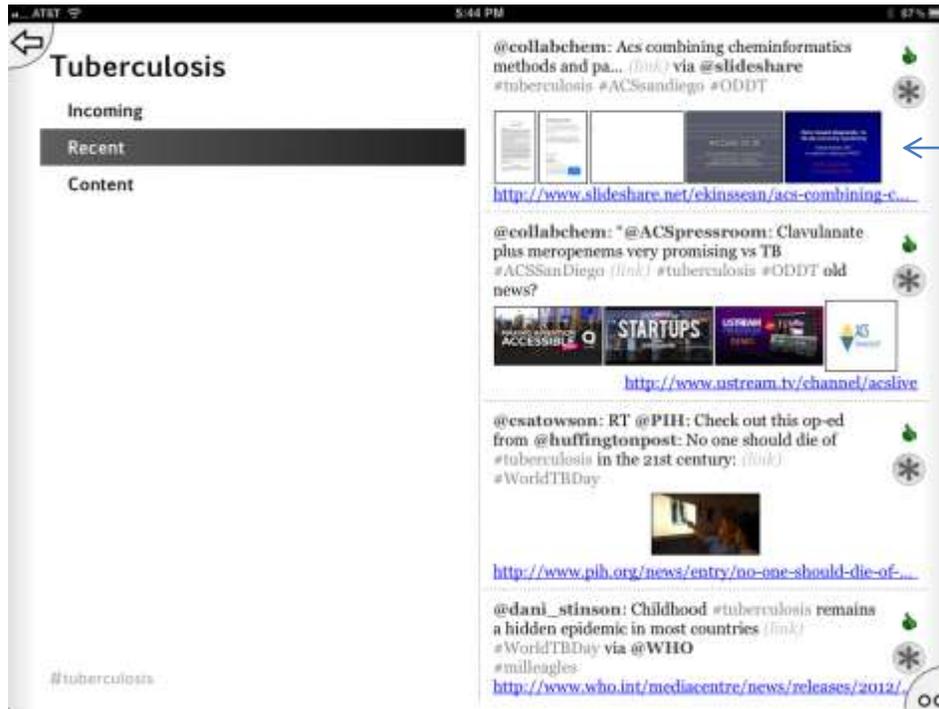


Fig. 4



Click on image to open it

Recent factoids with a vote count of +1 or better

Fig. 5

AT&T 9:44 AM 93%

Tuberculosis

Incoming
Recent
Content

Click on image to open it

Ranked content

Content is currently anything with a vote count of +1 or better, sorted by most popular first

@ODDTTest: (link) Known #tuberculosis drugs
<http://molsync.com/share/?src=http://dl.dropbox.com...>

@ODDTTest: (link) A series of #tuberculosis inhibitors
<http://molsync.com/share/?src=http://dl.dropbox.com...>

@TBmanifesto: RT @OperationASHA: One sneeze can release upto 40,000 droplets and each one can potentially cause infection #tuberculosis #healthcare #ngo (link)
<http://www.businessweek.com/news/2012-02-23/anci...>

#tuberculosis

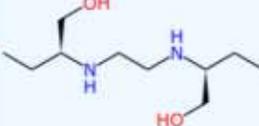
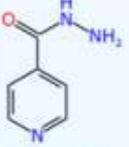
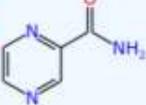
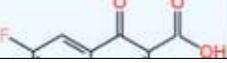
Fig. 6

Close 12:52 PM Not Charging

MolSync Sharing

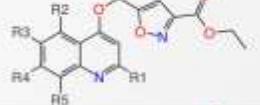
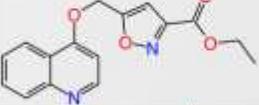
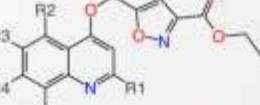
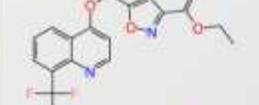
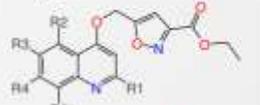
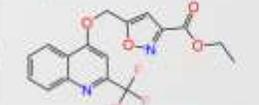
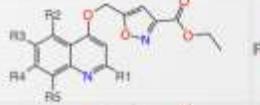
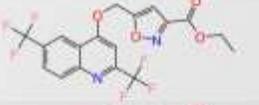
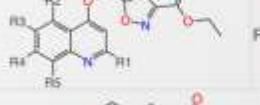
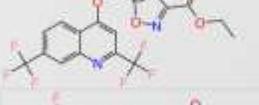
Download DataSheet

Tuberculosis drugs

	Molecule	Data
Row#1 Download		Name: ethambutol
Row#2 Download		Name: isoniazid
Row#3 Download		Name: pyrazinamid
Row#4 Download		

A

5:51 PM 89% BMS

	$R-H-R-H-R-H-R-H-R-H$		# 7a MABA MC: 25.1 μ M LORA MC: 13.2 μ M Vero IC50: > 128 μ M
	$R-H-R-H-R-H-R-H-R-F$		# 7b MABA MC: 10.6 μ M LORA MC: 56.6 μ M Vero IC50: > 128 μ M
	$R-F-R-H-R-H-R-H-R-H$		# 7c MABA MC: 3.2 μ M LORA MC: 25.1 μ M Vero IC50: > 128 μ M
	$R-F-R-H-R-F-R-H-R-H$		# 7d MABA MC: 0.7 μ M LORA MC: 7.6 μ M Vero IC50: > 128 μ M
	$R-F-R-H-R-H-R-F-R-H$		# 7e MABA MC: 1.3 μ M LORA MC: ml Vero IC50: > 128 μ M
	$R-F-R-F-R-H-R-H-R-H$		# 7f MABA MC: 9.8 μ M LORA MC: ml Vero IC50: > 128 μ M

B

Fig. 8

