Expanding Open Drug Discovery Teams: A New Mobile App for Scientific Collaboration

Sean Ekins[1] and Alex M. Clark[2]
[1] Collaborations in Chemistry, 5616 Hilltop Needmore Road, Fuquay Varina, NC 27526, U.S.A.
[2] Molecular Materials Informatics, 1900 St. Jacques #302, Montreal, Quebec, Canada H3J 2S1.

Introduction

Tools for drug discovery collaboration predominantly revolve around desktop computer applications[1, 2] though these authors believe that we will see a natural evolution toward the use of mobile apps in the drug discovery laboratory [3].

The Open Drug Discovery Teams (ODDT) project provides a mobile app primarily intended as a research topic aggregator of predominantly open science data collected from various sources on the internet. It exists to facilitate interdisciplinary teamwork and to relieve the user from data overload, delivering access to information that is highly relevant and focused on their topic areas of interest. Research topics include areas of chemistry and adjacent molecule-oriented biomedical sciences, with an emphasis on those which are most amenable to open research at present. These include rare and neglected diseases, and precompetitive and public-good initiatives such as green chemistry.

The ODDT project uses a free mobile app as user entry point. The app has a magazine-like interface, and server-side infrastructure for hosting chemistry-related data as well as value added services. The project is open to participation from anyone and provides the ability for users to make annotations and assertions, thereby contributing to the collective value of the data to the engaged community. Much of the content is derived from public sources, but the platform is also amenable to commercial data input. The technology could also be readily used in-house by organizations as a research aggregator that could integrate internal and external science and discussion. The infrastructure for the app is currently based upon the Twitter API as a useful proof of concept for a real time source of publicly generated content. This could be extended further by accessing other APIs providing news and data feeds of relevance to a particular area of interest. As the project evolves, social networking features will be developed for organizing participants into teams, with various forms of communication and content management possible.

Methods

Client app. The primary user interface is via the ODDT app, for iOS-based devices (iPhone, iPod and iPad). The app provides a user interface that is inspired by the "magazine-like" Flipboard app: the user initially selects from a list of topics, and from there can flip through recently posted content. The app is free for anyone to use, and provides content-consumption features as its primary purpose. As it evolves, the app will also be used to participate in active content-sharing and social networking activities.

Server. The server-side architecture is based on the *com.mmi* software stack, used by the *molsync.com* service, which currently provides additional cheminformatics capabilities for various mobile apps.[39] The extensions designed to host the ODDT project make use of Twitter as the primary source of content, which is regularly polled and assimilated into the data collection. The service provides an API for accessing ODDT topics and content. As the project evolves, the server will be gradually augmented to recognize particular data sources and information streams, and provide value added functionality. Currently it is able to recognize chemical data such as molecular structures, reactions and datasheets.

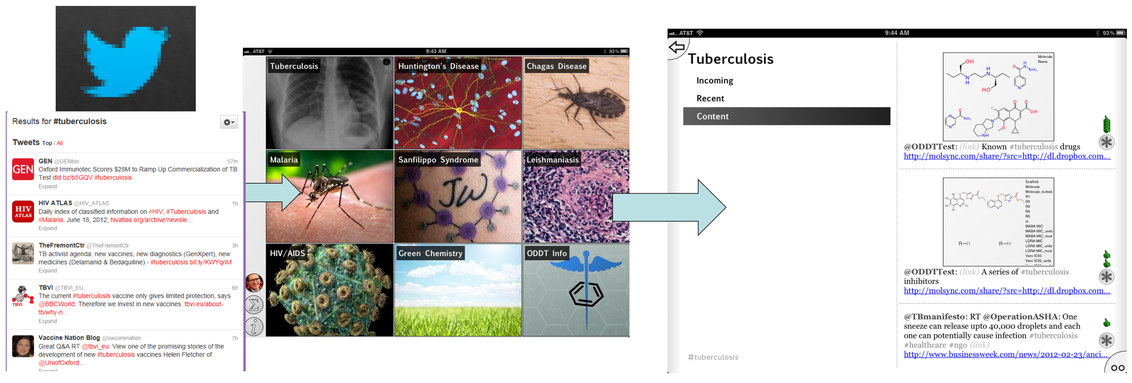

Fig 1. Capturing information from Twitter for select hashtags then viewing content and endorsing or disapproving in app. The app is chemistry aware so molecules and SAR tables can be visualized in the App.

Acknowledgement

We kindly acknowledge Antony Williams for suggesting integration of Google Alerts and we thank our alpha testers.

Results

We have defined a small number of topics, corresponding to Twitter hashtags such as: #tuberculosis, #malaria, #hivaids, #huntingtons, #sanfilipposyndrome, #leishmaniasis, #chagas, #h5n1 #hhf4gan and #greenchemistry. We have built the server architecture for harvesting URLs from these tweets, and gathered them together into a collection that can be accessed via an API. We have performed some minimal recognition of the links and, in particular, annotated those which lead to chemical data content, as well as enumerating a list of embedded images within the corresponding web page (Fig 1). We have also hosted the server on molsync.com initially, with the intention of relocating at a later date.

Discussion

Since the release of ODDT we have added #h5n1 and #hh4gan. In order to expand further we have launched an IndieGoGo crowdfunding campaign to fund expansion of ODDT (http://www.indiegogo.com/projects/122117). This will fund servers for 3 years to keep ODDT free and also integration of additional datasources on disease topics (Fig 2). These additional datasources should greatly increase the content of the app and increase its value for scientific collaboration and discovery.

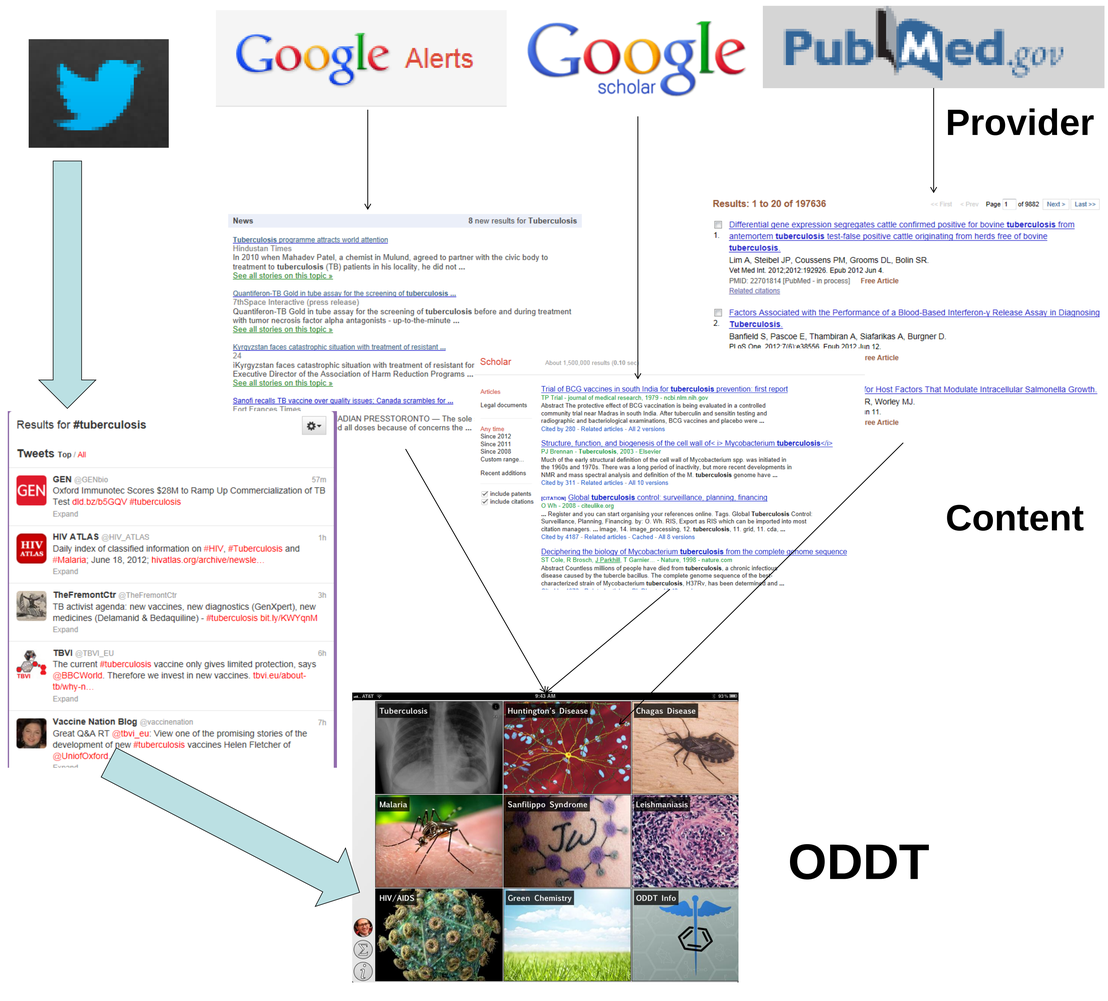

Fig 2. Capturing information additional data sources in future (thin arrows).

References

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