Using The Open Drug Discovery Teams (ODDT) Mobile App To Bring Molecules & SAR From Behind Journal Paywalls

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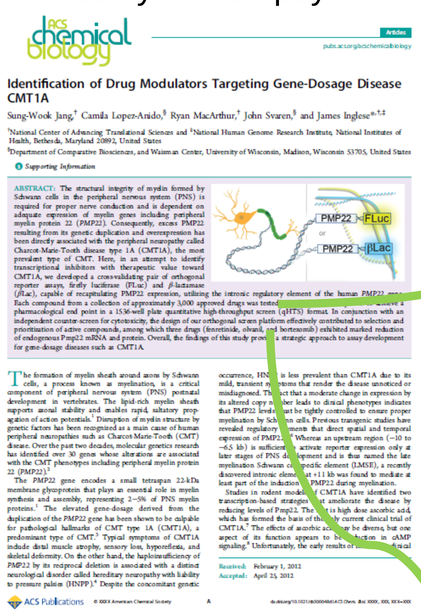
What is The problem?

Research funded by the tax-payer is locked behind journal paywalls. In most cases many researchers are interested in a few key pieces of information. Drug discovery scientists want to see molecule structures and structure activity relationship data. In the absence of mandates that require the immediate release of tax-payer funded research into the research commons, or the requirement that journals deposit data with such manuscripts into open databases, we now propose a novel approach. As people read scientific papers they can simply tweet molecule related information from the paper like a molecule structure (by using an app to draw it, or retrieve it from a database like ChemSpider) or name, and using mobile apps such as “SAR Table” they can also create SAR tables and tweet these to the appropriate disease community. Data can be freed from behind paywalls.

The Open Drug Discovery Teams (ODDT) project uses a free mobile app as user entry point **http://tinyurl.com/6l9qy4f**. 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. The infrastructure for the app is currently based upon the Twitter API and uses Google Alerts RSS feeds as a useful proof of concept for a real time source of publicly generated content.

We now highlight how ODDT can be used to share molecules and SAR data with the research community and general public by tweeting this information as they read a paper with the appropriate hashtag for the disease topic. This could be a valuable asset for the scientific community and release data that is inaccessible to many scientists and patients. In the absence of mandates to free up data it may be possible to use crowdsourcing to deposit such small but important fragments of molecule related information into the public domain.

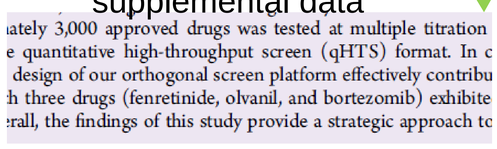
An example of an article behind a paywall that was funded by the tax-payer


ACS Chemical Biology

Identification of Drug Modulators Targeting Gene-Dosage Disease CMT1A

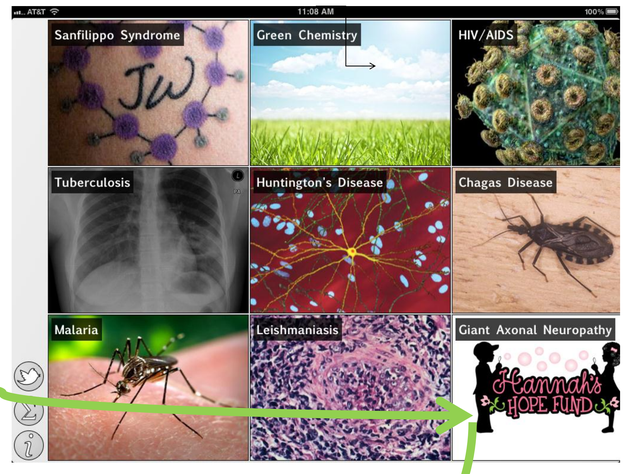
Sung-Wook Jang,† Camila Lopez-Arido,§ Ryan MacArthur,† John Svaren,§ and James Inglese*,†,‡

abstract -describes 3 active compounds found by HTS screening –structures only in supplemental data

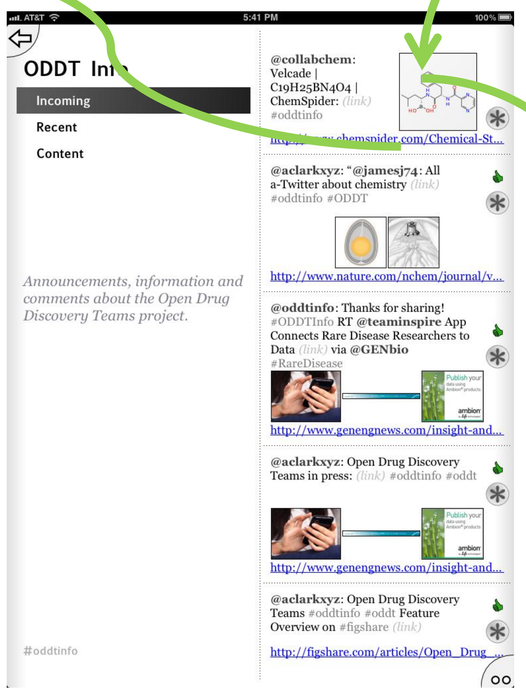

…ately 3,000 approved drugs was tested at multiple titration
…e quantitative high-throughput screen (qHTS) format. In c
… design of our orthogonal screen platform effectively contribu
…h three drugs (fenretinide, olvanil, and bortezomib) exhibite
…erall, the findings of this study provide a strategic approach to

Tweet each molecule from ChemSpider with a hashtag for disease or other topic

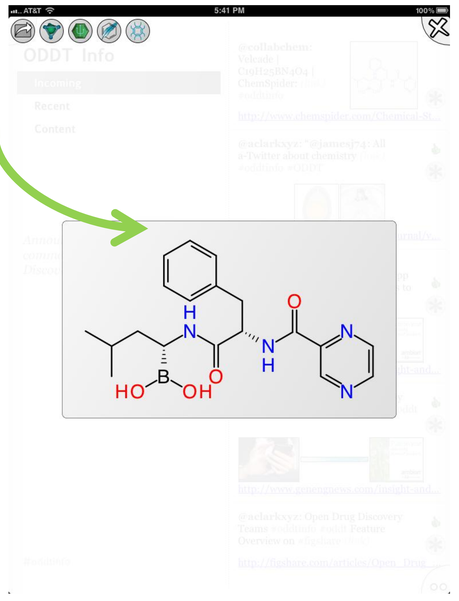
Disease topic followed in the ODDT app



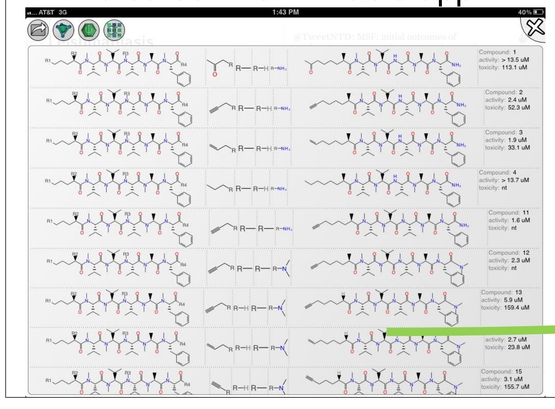
Molecules collected in app

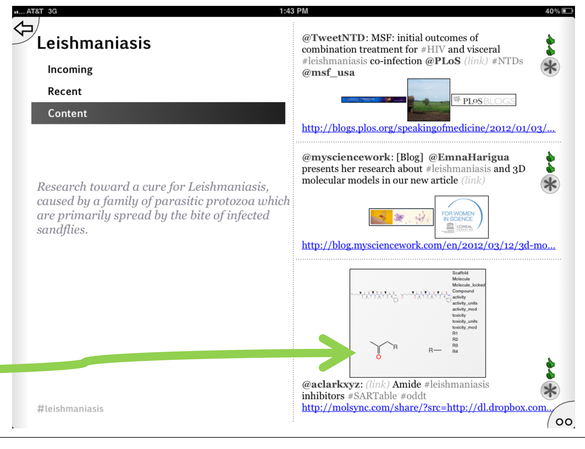


User can click on link to open in app or click on URL to open in original source



SAR from papers can also be created in SAR Table app





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