

Secure Sharing with Mobile Cheminformatics Apps Followed by Open Publication When Ready

Sean Ekins¹ and Alex M. Clark²

¹ Collaborations in Chemistry, 5616 Hilltop Needmore Road, Fuquay Varina, NC 27526, U.S.A., ² Molecular Materials Informatics, Montreal, Quebec, Canada H3J 2S1.

Secure sharing of molecules and bioactivity data using mobile apps.

The technologies already exist that enable the scientist to securely share molecule structures or structure-activity relationship (SAR) tables for multiple molecules with one or more other scientists (perhaps even a group). This can be done for a very small investment. We now describe how just 2 commercial cheminformatics apps can enable such sharing **at very reasonable cost (\$25)**.

SAR Table: A specialized editor for building tables containing an homologous series of scaffolds and substituents, creating composite structures, and providing activity data. Can be used to prepare figures for manuscripts, or to recreate data from the literature. **MolSync:** A chemistry-aware client for remotely stored files hosted by *Dropbox*. Provides viewing and editing capabilities, as well as serving as an intermediary for sharing content with other apps. It can also be used to explicitly synchronize data with other apps.

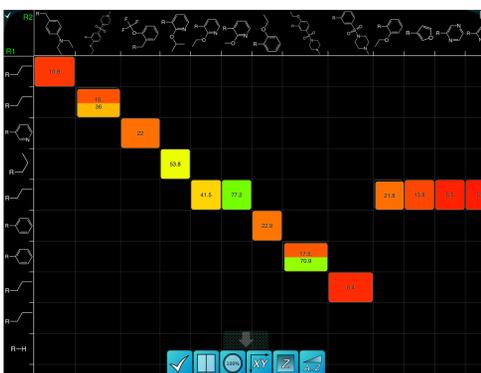
Molecules can be sketched in **SAR Table** and then shared via **MolSync**. **MolSync** enables files to be readily deposited in *DropBox* folders. This cloud-based storage facility provides a free capability to share (securely) limited amounts of data with selected individuals. This approach represents a very cost effective way to enable secure chemistry and bioactivity data sharing.

When data is ready to be shared openly a third mobile app can be used. The **Open Drug Discovery Teams (ODDT)** project uses a free mobile app as the user entry point <http://tinyurl.com/6I9qy4f>. 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. Using Twitter, users can easily push data from **SAR Table** or **MolSync** into **ODDT**.

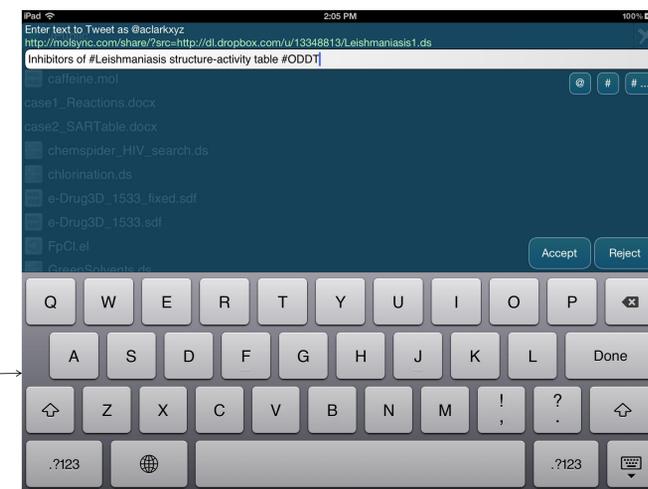
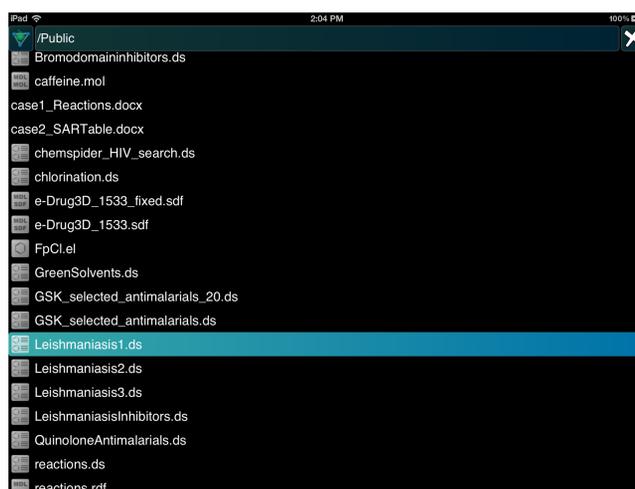


Showing molecule and bioactivity data export to Molsync

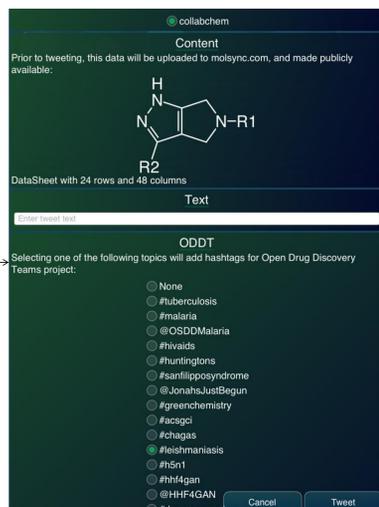
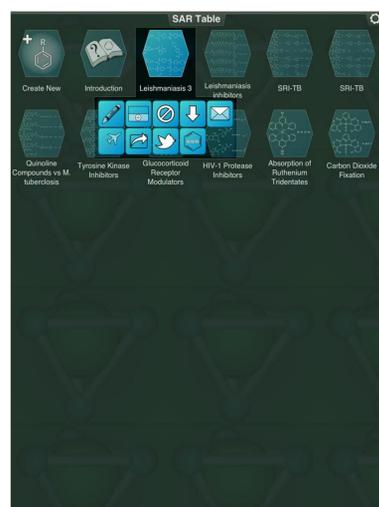
Scaffold	R1	R2	R3	Molecule	Molecule No.	CDD Number	Average	Inhibitor
					NEU-000001	CDD-1375763	10.8	100
					NEU-000010	CDD-957450	20	100
					NEU-000016	CDD-1375765	22	100
					-0000020	CDD-1377409	53.8	100
					-0000021	CDD-1377410	41.5	100



Showing data in Dropbox and how its limited access

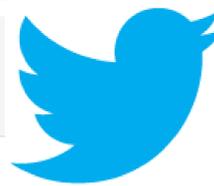


Showing how when ready, a subset or all data can be tweeted to ODDT



When ready for public sharing push to ODDT

Content from web
Google Alerts



User tweets with #leishmaniasis

Links to papers, blogs, websites

