Subject: chembl server
Posted by pc419714@ohio.edu on Sun, 13 Oct 2019 17:30:41 GMT
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I'm building a QSAR creator in python. https://www.aidrugdiscovery.net

We are trying to figure out how you communicated with the Chembl server to download compounds from the target name. Are you aware of any python clients that allow you to do this with Chembl? We're looking at your source code-- ChemblCommunicator.java, ChemblServerConstants.java, DETaskChemblQuery.java

There's pugrest for pubchem. I don't see any easy way of communicating with either pubchem or chembl to download the compounds based on their target. We might just tell our clients to download Data Warrior in order to get the compounds.... (or maybe create a Data Warrior plugin that allows you to communicate with our toolkit). Maybe a data warrior plugin that piped the compounds to our QSAR creator. If you had any thoughts on our concept, I'd love to hear.

Loving Data Warrior, defending my masters thesis using it. Thanks so much for your great software and answering all my questions!

Patrick Chirdon

Subject: Re: chembl server
Posted by thomas on Mon, 21 Oct 2019 19:13:51 GMT
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DataWarrior is accessing a copy of the Chembl database on openmolecules.org.
This server is optimized for fast structure search and result retrieval and is accessible via http.

For your purpose the fastest approach would probably be to download the Chembl database in MySQL,
install it on your server and access it via SQL language. From python this should be possible.

Alternatively, as you suggest, you may, of course, use DataWarrior for target specific downloads.
DataWarrior plugins are meant for getting data into DataWarrior, not for export.

Thomas

Subject: Re: chembl server
Posted by pc419714@ohio.edu on Sat, 02 Nov 2019 16:07:19 GMT
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I think what we will probably do is launch Data Warrior from our application. I think this should be possible.