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