Subject: Re: chembl server

Posted by thomas on Mon, 21 Oct 2019 19:13:51 GMT

View Forum Message <> Reply to Message

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