Subject: pchembl values
Posted by evehom on Tue, 24 Nov 2020 09:52:53 GMT
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Hi,

The ability to import data directly from ChEMBL is great, but the reported Units (nM, %, mM etc) can be very mixed, and require filtering and conversion. Would it be possible to add (join) the pchembl_value field from the activities table in ChEMBL, as this is a standardized activity value that could be used straight off for (Q)SAR analyses?

Thanks/Evert

Subject: Re: pchembl values
Posted by thomas on Thu, 26 Nov 2020 12:28:19 GMT
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this absolutely makes sense. I am currently updating to Chembl27 and check whether I can include the pvalue without sacrificing compatibility to older DataWarrior installations.

Subject: Re: pchembl values
Posted by thomas on Sat, 28 Nov 2020 23:08:10 GMT
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Now the server is updated to use Chembl27 and to provide pValues. To retrieve them you need to use the newest DataWarrior development patch, which is downloadable from the download page after clicking 'read and understood'. The link is in the fine print!