Subject: Re: Importing compounds with assay data from Pubchem into Datawarrior
Posted by thomas on Thu, 19 Aug 2021 18:56:03 GMT
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Hi Jon and Norwid,

I can confirm that Jon's URL now works, but I remember I had trouble before.
Structure retrieval based on names is the second best solution, although the openmolecules server knows most of the PubChem names unless they are very long.

If you can get an SD-File with SIDs or CIDs, the result will be more complete and potentially may have less errors.

Thomas