Subject: Batch conversion of dwar files
Posted by jeremy on Wed, 21 Oct 2020 15:19:10 GMT
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Hello,
I have to convert a bunch of dwar files into csv (or SDF) files.
I can open them one at a time and export; but I would prefer a more automated way. I can read the dwar file as tab delimited files (ignoring top lines), but I don't know how to convert the structure string into a molecule. Is there a way to convert the structure string into a molecule outside DW?
Thank you