
Subject: Can you disable SMILES conversion?

Posted by [zsolt](#) on Mon, 07 Dec 2020 11:40:06 GMT

[View Forum Message](#) <> [Reply to Message](#)

a quick question on SMILES conversion: using DataWarrior with some larger datasets we noticed that SMILES conversion takes an unacceptably long time. For certain workflows it is not required for us so would like to ask if it is possible to disable it?

Another idea I am thinking as a workaround is to somehow craft a DataWarrior specific file (e.g. a .dwar) where I specify the columns containing my SMILES as plain text type - maybe then DataWarrior won't try converting it. (However I would not like to have to specify all the extra bits that are contained in the .dwar file like the position of the windows, filters etc...)

Thanks in advance,
Zsolt
