
Subject: Re: Can you disable SMILES conversion?
Posted by [thomas](#) on Tue, 08 Dec 2020 16:30:29 GMT

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If you just give your TAB delimited text file the '.dwar' extention, then DataWarrior doesn't try to convert SMILES codes. A content sample would be: (your file could even contain chemical structure as idcodes, which would be recognized, if the column name ends with '[idcode]')

ID Smiles
1 CCOCC
2 CCCO
3 CCO
