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

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

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
