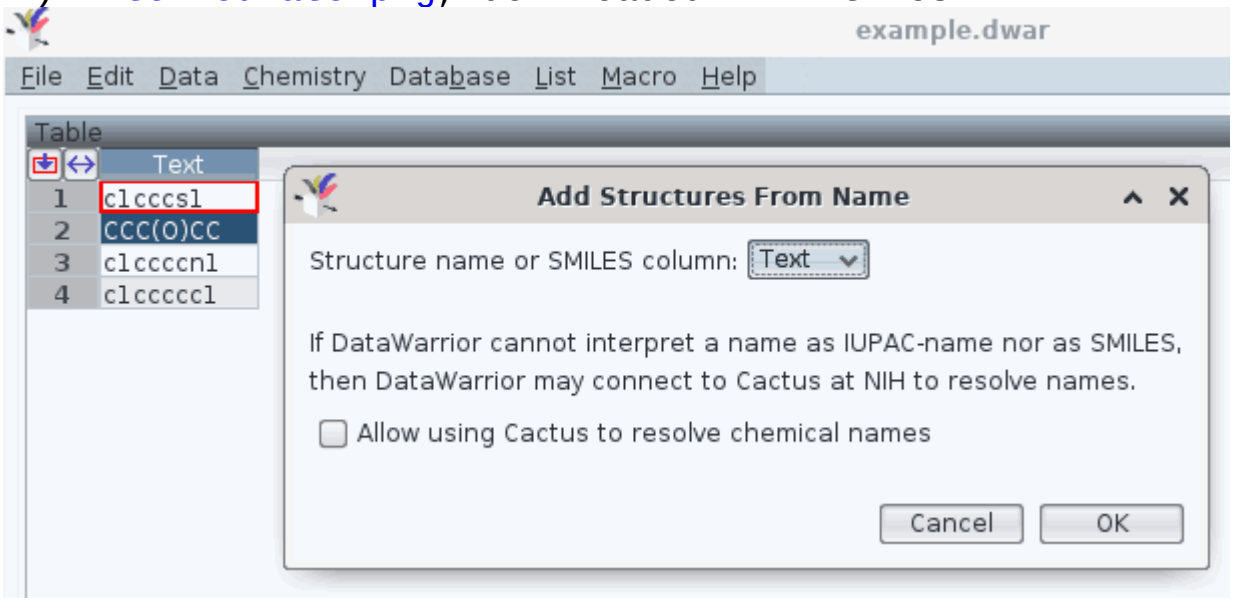
Subject: Re: Smiles to Structure
Posted by nbehrnd on Fri, 24 Jul 2020 09:01:04 GMT
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Let's say you have a text column with the SMILES strings for which you want to see as the 2D structures. With Chemistry -> Add Structure From Name, a new menu will be shown to you where you specify the column DW shall access for this processing. As intended, this then will consider all of the entries at once with the generation of an additional column.

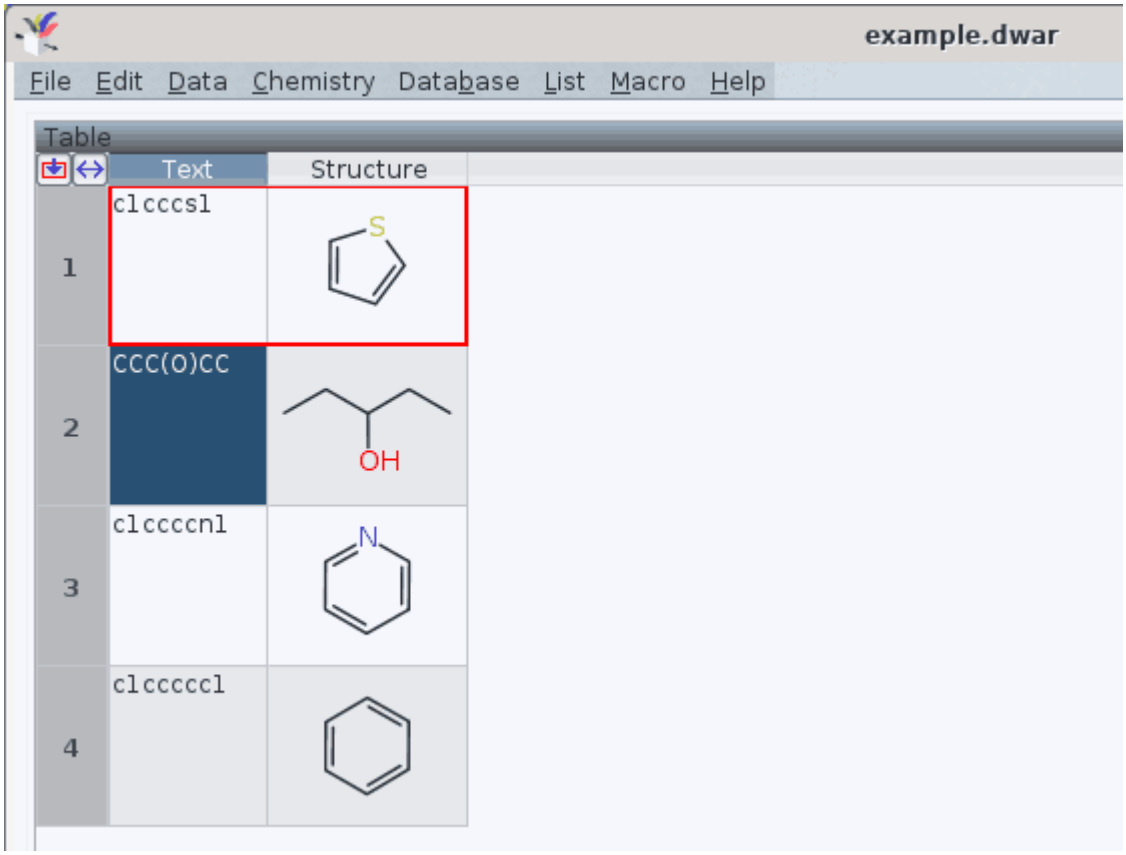
Norwid

File Attachments

1) example.dwar, downloaded 791 times
2) intermediate.png, downloaded 1127 times



3) result.png, downloaded 1005 times


example.dwar
File Edit Data Chemistry Database List Macro Help
Table
Text
Structure
1
clcccsl
S
2
CCC(O)CC
OH
3
clccccnl
N
4
clcccccl