
Subject: Re: Smiles to Structure

Posted by [nbehrnd](#) on Fri, 24 Jul 2020 09:01:04 GMT

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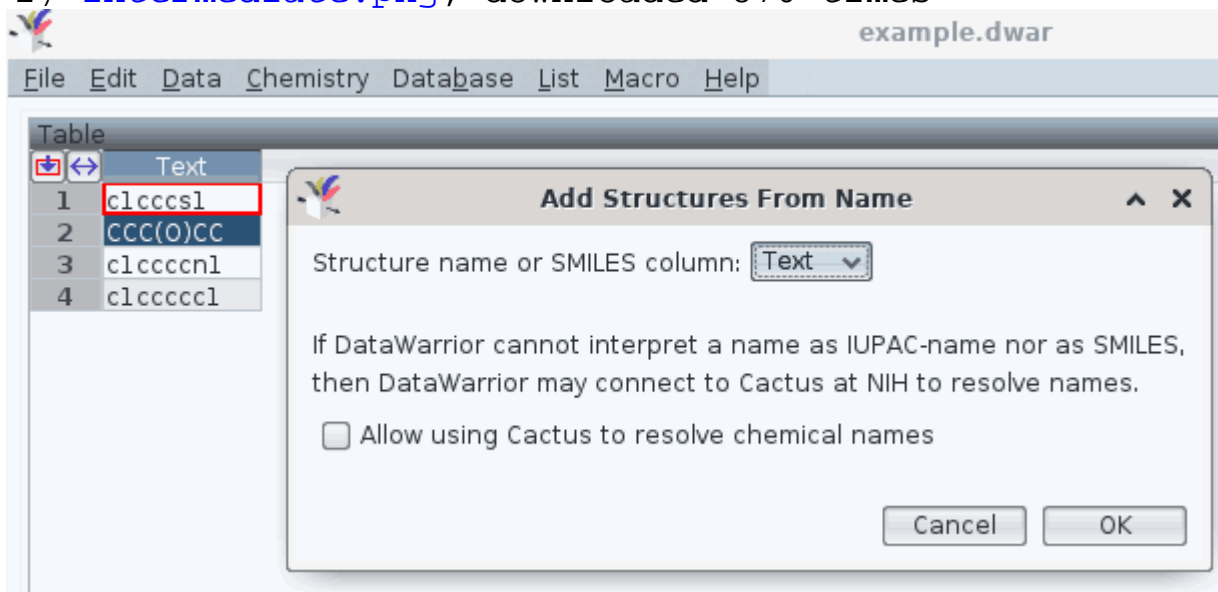
Let's say you have a text column with the SMILES strings for which you want to see as the 2D structures. With Chemistry -> Add Structure From Name, a new menu will be shown to you where you specify the column DW shall access for this processing. As intended, this then will consider all of the entries at once with the generation of an additional column.

Norwid

File Attachments

1) [example.dwar](#), downloaded 709 times

2) [intermediate.png](#), downloaded 870 times


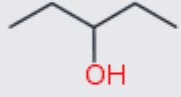
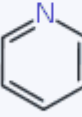


3) [result.png](#), downloaded 773 times

example.dwar

File Edit Data Chemistry Database List Macro Help

Table

	Text	Structure
1	<chem>c1cccs1</chem>	
2	<chem>CCC(O)CC</chem>	
3	<chem>c1cccn1</chem>	
4	<chem>c1ccccc1</chem>	