Subject: Smiles to Structure
Posted by sbembenek18 on Fri, 24 Jul 2020 06:10:47 GMT

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I have a Smiles column that I would like to display as the actual structures. So, I created a structure column (one already exists) and attempted to past the smiles column into the structures column but to no avail. I know such a thing is possible one at a time, but I'd like to accomplish this all at once.

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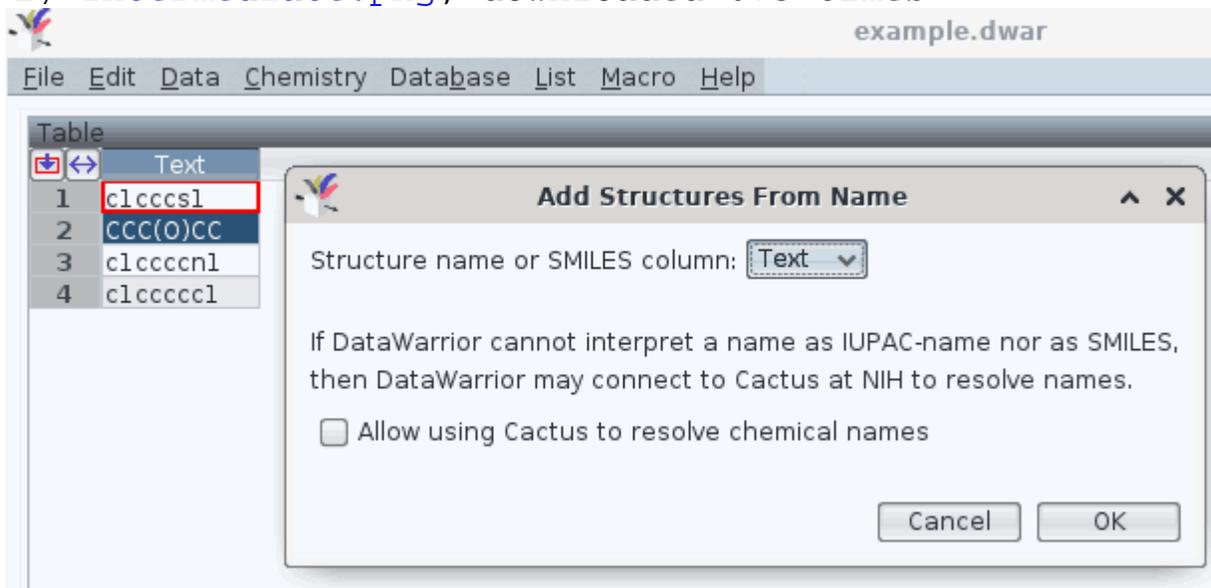
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Let's say you have a text column with the SMILES strings for which you want to see as the 2D structures. With Chemistry -> Add Structure From Name, a new menu will be shown to you where you specify the column DW shall access for this processing. As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

Norwid
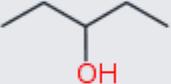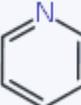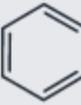
File Attachments
1) example.dwar, downloaded 649 times
2) intermediate.png, downloaded 673 times

3) result.png, downloaded 604 times

example.dwar

File Edit Data Chemistry Database List Macro Help

Table

	Text	Structure
1	clcccs1	
2	CCC(O)CC	
3	clccccn1	
4	clccccc1	

Subject: Re: Smiles to Structure
Posted by thomas on Sat, 15 Aug 2020 09:08:39 GMT
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Thank you very much for this question. It makes, of course, a lot of sense being able to paste a list of SMILES, IUPAC names, or common names into an existing structure column. I have added this behaviour to the current development version, which is also downloadable from the home page.

Subject: Re: Smiles to Structure
Posted by sbembenek18 on Mon, 17 Aug 2020 20:25:38 GMT
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thanks

Subject: Re: Smiles to Structure
Posted by sbembenek18 on Mon, 17 Aug 2020 20:28:23 GMT
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thanks