
Subject: Re: Row wise chemical reaction
Posted by [nbehrnd](#) on Tue, 17 Dec 2019 10:22:29 GMT
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Hello Patrick,

I understand your aim is to bring line wise structures deposit in independent columns into a cell in common.

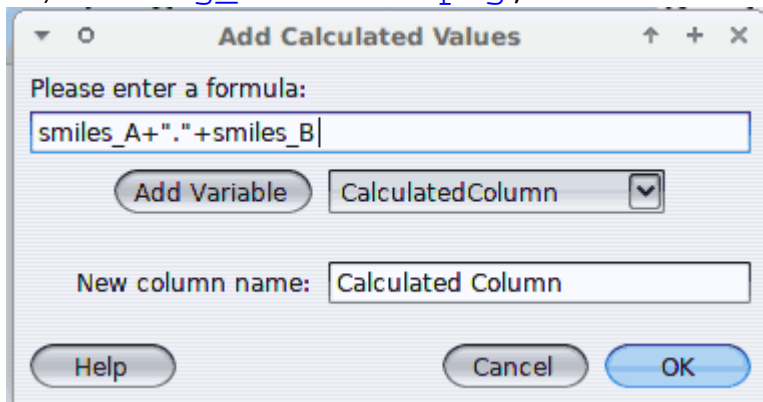
If so, 1) convert the structures you already have in the .dwar file as SMILES. You find this function along chemistry -> from chemical structure -> Add SMILES code, to be applied for each column of structures. 2) To concatenate the SMILES, reach for Data -> Add Calculate Values. In the new sub-menu, you define a string addition, of the SMILES, as shown below:

After confirmation by «ok», DataWarrior creates a new column with the result. You then 3) convert the concatenated SMILES string into a sketch with Chemistry -> Add Structures From Name. This equally creates a new column, with both molecules represented in one cell:


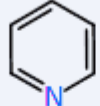
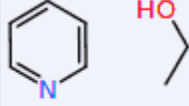

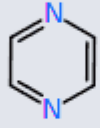
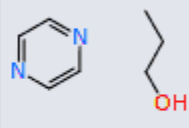

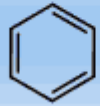
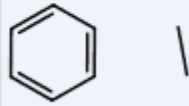
Norwid

File Attachments

1) [string_addition.png](#), downloaded 1705 times



2) [example.png](#), downloaded 1834 times

	structure_A	smiles_A	structure_B	smiles_B	Calculated Column	Structure
1		CCO		c1ccncc1	CCO.c1ccncc1	
2		CCCO		c1cnccn1	CCCO.c1cnccn1	
3		CC		c1ccccc1	CC.c1ccccc1	

3) [MWE_joining_structures.dwar](#), downloaded 770 times