

Subject: Re: How to perform general R group searches in DW

Posted by [nbehrnd](#) on Tue, 11 Jan 2022 06:06:19 GMT

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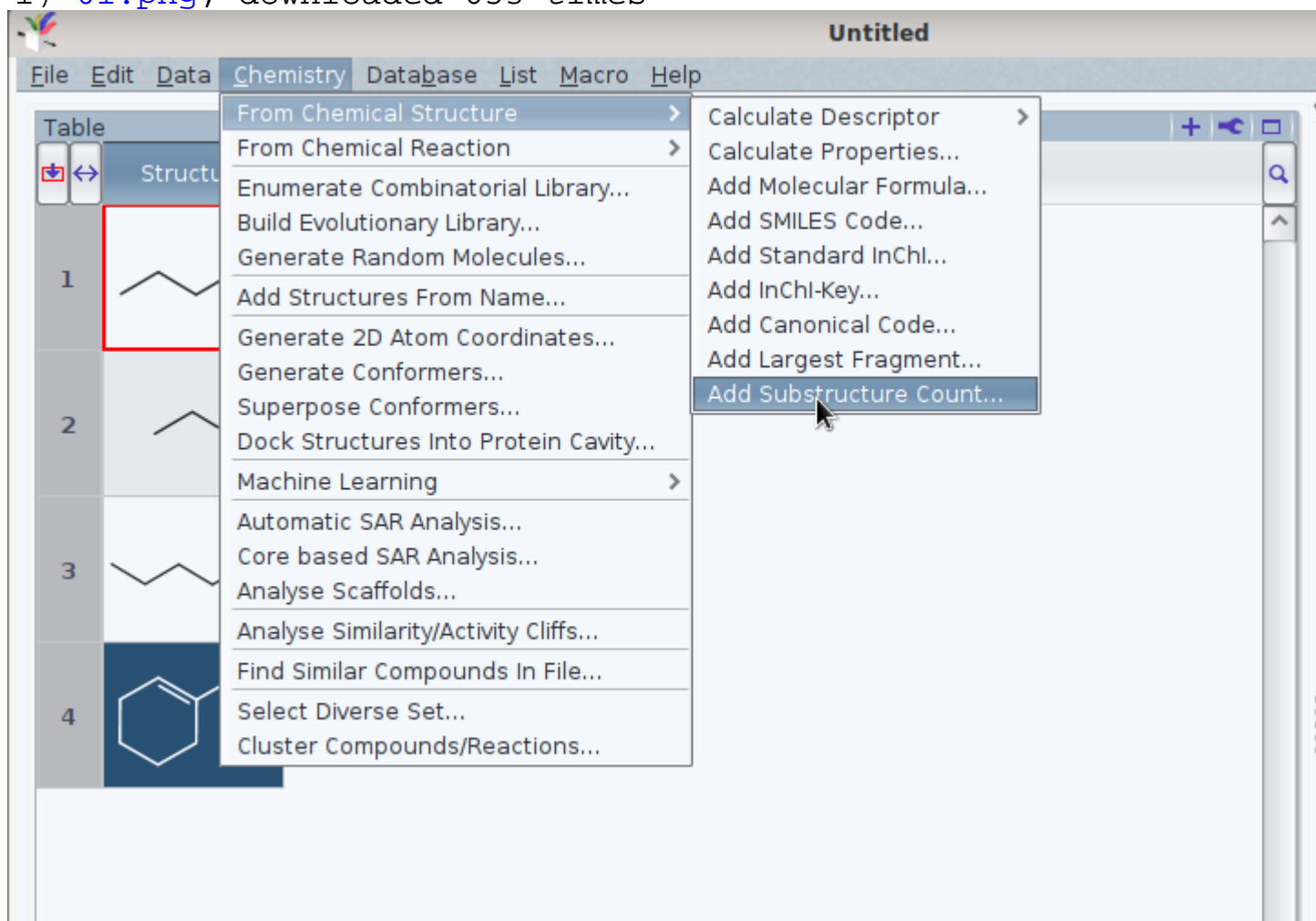
Dear JonW,

at least the nightly-builds version of DW contains a function to define a substructure query. Follow Chemistry -> From Chemical Structure -> Add Substructure Count to open a new instance of the sketcher, and decide in favour/against the criterion of overlapping substructure matches. In the matrix view, you obtain a new column with the number of occurrences of the pattern; at the right hand side, there will be a new slide ruler to filter the display. By substructure, one may define queries permitting more than one atom type on one site, too:

Norwid

File Attachments

1) [01.png](#), downloaded 653 times




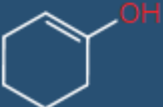


2) [02.png](#), downloaded 718 times

Untitled

File Edit Data Chemistry Database List Macro Help


Table

	Structure
1	
2	
3	
4	

Add Substructure Count

Structure column:

Column Name:

Structure: 

Include overlapping substructure matches


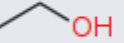

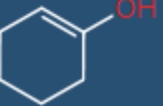
Help Cancel OK

3) 03.png, downloaded 694 times

Untitled

File Edit Data Chemistry Database List Macro Help

Table

	Structure	Substructure Count
1		1
2		0
3		1
4		1

Substructure Count

0 1

4) 04.png, downloaded 1418 times

The screenshot shows a software window titled "Untitled" with a menu bar containing "File", "Edit", "Data", "Chemistry", "Database", "List", "Macro", and "Help". Below the menu bar is a "Table" with four rows. The first row is selected and highlighted in blue, and its cell contains a chemical structure of a six-membered ring with one oxygen atom (tetrahydropyran), which is also enclosed in a red rectangular box. The second row contains a six-membered ring with two oxygen atoms (1,3-dioxane). The third row contains a six-membered ring with one nitrogen and one oxygen atom (piperidine). The fourth row contains a simple six-membered carbon ring (cyclohexane). Overlaid on the right side of the table is a dialog box titled "Add Substructure Count". The dialog box has a "Structure column:" dropdown menu set to "Structure" and a "Column Name" text box containing "Substructure Count". Below these is a large text area labeled "Structure" containing the chemical structure [C,N]O. At the bottom of the dialog box, there is an unchecked checkbox labeled "Include overlapping substructure matches" and three buttons: "Help", "Cancel", and "OK".