

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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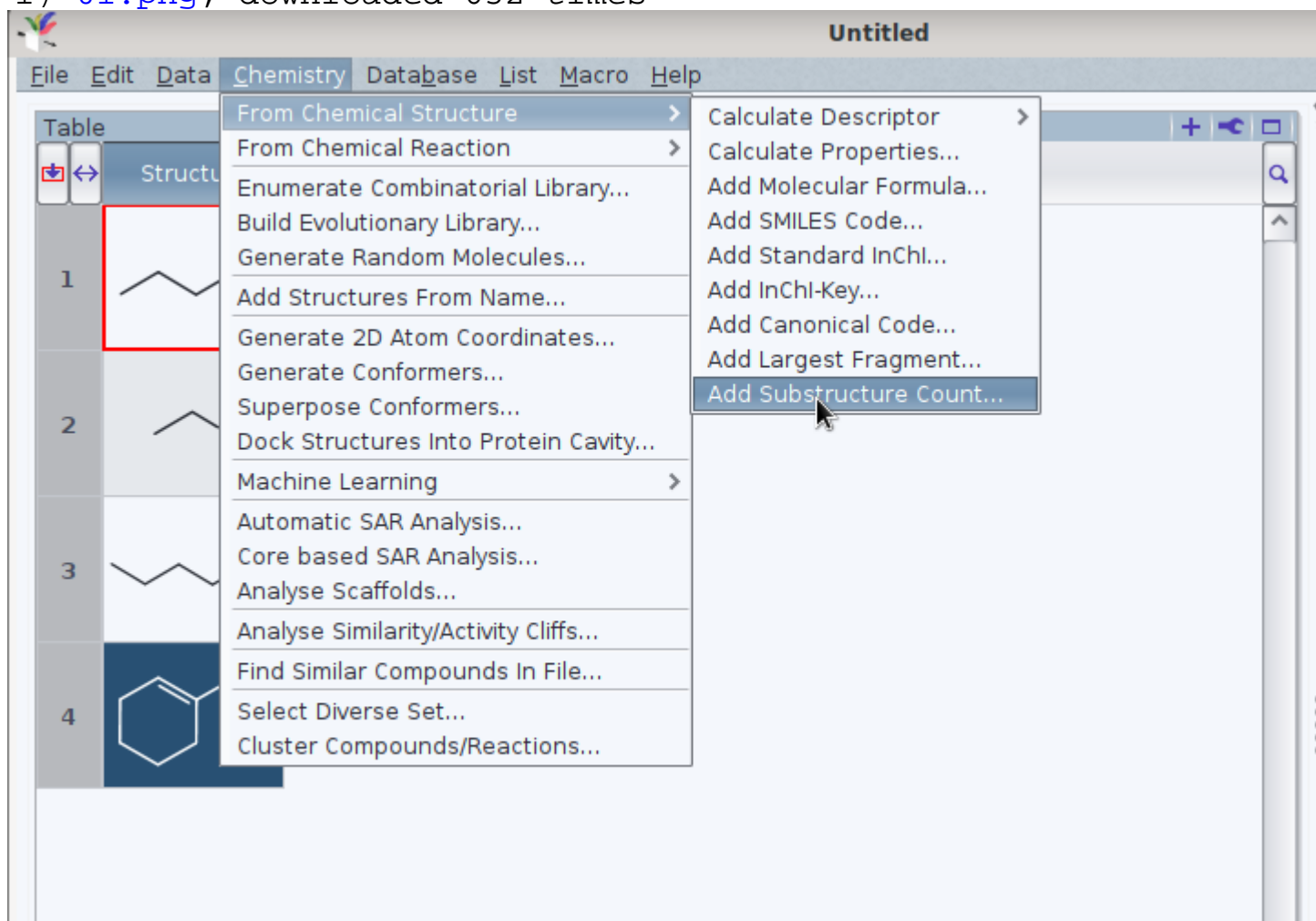
Dear JonW,

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 652 times




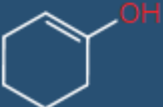


2) [02.png](#), downloaded 717 times

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


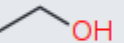

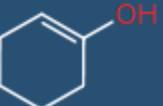
Help Cancel OK

3) 03.png, downloaded 693 times

Untitled

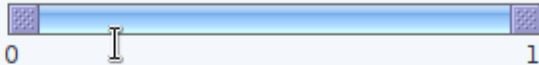
File Edit Data Chemistry Database List Macro Help

Table

	Structure	Substructure Count
1		1
2		0
3		1
4		1

Substructure Count

0 1



4) 04.png, downloaded 1417 times

The screenshot shows a software window titled "Untitled" with a menu bar (File, Edit, Data, Chemistry, Database, List, Macro, Help). Below the menu is a "Table" with four rows. The first row is selected and highlighted with a red border. The structures in the rows are: 1. A six-membered ring with one oxygen atom (tetrahydropyran). 2. A six-membered ring with two oxygen atoms (1,4-dioxane). 3. A six-membered ring with one nitrogen and one oxygen atom (piperidine). 4. A plain six-membered carbon ring (cyclohexane).

An "Add Substructure Count" dialog box is open over the table. It has the following fields and options:

- Structure column: **Structure** (dropdown menu)
- Column Name: **Substructure Count** (text input)
- Structure: [C,N]O (text input with a chemical structure icon)
- Include overlapping substructure matches
- Buttons: Help, Cancel, OK