
Subject: Re: Saving 2D-structure with labels
Posted by [nbehrnd](#) on Thu, 30 Jun 2022 18:03:12 GMT
[View Forum Message](#) <> [Reply to Message](#)

Dear Vijay,

congratulations to your publication.

Note, table 1 includes some examples of «counting patterns» which indeed exceed DW's set of pre-set statistics (e.g., counting small saturated carbon-only cycles) available via chemistry -> from chemical structure -> calculate properties. However, the development version of DW offers an additional functionality via chemistry -> from chemical structure -> add substructure count. Assisted by the program's sketcher, you may define countable pattern matching your needs like «excluding S of sulfone, the eighth atom should be an aromatic carbon atom»

By selection (lasso) and double click, the properties of the atoms in question may be specified further. The documentation calls this «substructure count»,^[1] just prior to the section header «The Structure Filter».

With best regards,

Norwid


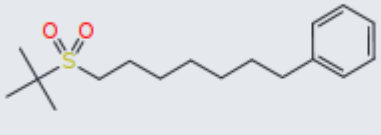
[1] <https://openmolecules.org/help/chemistry.html#StructureFilter>

File Attachments

1) [special_count_sulfone.png](#), downloaded 1720 times

File Edit Data Chemistry Database List Macro

Table


	Structure	Substructure Count
1		0
2		1

Add Substructure Count

Structure column:

Column Name

Structure



Include overlapping substructure matches

Help Cancel OK

- 2) [special_count_sulfone.dwar](#), downloaded 580 times
- 3) [atom_features.png](#), downloaded 685 times

Atom Query Features ^ X

Any atomic number

Allowed atoms:

Aromaticity:

Ring bonds:

Smallest ring size:

Any ring size:

Charge:

Non-H neighbours:

Hydrogen count:

Pi-electron count:

prohibit further substitution

require further substitution

match stereo center

is part of exclude group