Subject: Re: Saving 2D-structure with labels
Posted by nbehrnd on Thu, 30 Jun 2022 18:03:12 GMT
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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#StructureFilte r

File Attachments

1) special_count_sulfone.png, downloaded 602 times
2) special_count_sulfone.dwar, downloaded 119 times
3) atom_features.png, downloaded 130 times