Subject: Re: Filter out nasty functions
Posted by nbehrnd on Sun, 14 May 2023 20:24:37 GMT
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Dear Julio,

I would like to add two suggestions; how the task is presented/shared, and a revision of the SMILES string.

a) After recording a DW macro, it is possible to export this via Macro -> Export Macro as a file with file extension .dwam. This offers the advantage for an easier/faster import to replicate your observations (Macro -> Import Macro in a first step, Macro -> Run Macro to apply the instructions) by any subsequent reader of your post, because it typically is small enough to be attached to a message here (up to five files in total [e.g. incl. a small test data set] for a maximum over all files of 2MB). It equally prevents the omission of lines; in your most recent example, the opening how the macro is named (for the display within the DW session) and closing line </macro> was missing.

For the purpose of illustration, I enclose a small test set .dwar, and a macro to assign SMILES and compute Mw as .dwam.

b) Curious about the structure the SMILES strings describes, I relayed it to openbabel to write a .sdf, however without success.

```
$ obabel -:"Nc1c([C@@H](CC(C2=CNC(Nc3ccccc3)=CC2=O)=O)C(C(O[C@@H]2[C@@H]
3CCCC2)=O)=C3O)cccc1" -h --gen3d -O test.sdf -xv3000
============================
*** Open Babel Warning  in ParseSmiles
  Invalid SMILES string: 2 unmatched ring bonds.

0 molecules converted
```

Because equally ChemDraw test site[1] faces difficulties to process this one (Structure -> Load SMILES), as well as CDK Depict,[2] can you please check if the SMILES string shared contains the complete information?

With regards,

Norwid

[1] https://chemdrawdirect.perkinelmer.cloud/js/sample/index.htm l#
[2] https://www.simolecule.com/cdkdepict/depict.html

File Attachments

1) 10Random_Molecules.dwar, downloaded 375 times
2) compute_SMILES_Mw.dwam, downloaded 368 times