
Subject: suggest: adjustment .sdf export

Posted by [nbehrnd](#) on Fri, 15 May 2020 15:59:41 GMT

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Prior to further analysis of a library,[1] its entries were deduplicated by Data -> merge equivalent rows, using content of the structure column as sole criterion. The work with the .sdf subsequently generated by DataWarrior worked fine if the compound name column used the row number.

Yet, retaining the information of the molecules' name -- here, a PubChem identifier -- may be useful as a structure may be attributed more than one.[2] The corresponding choice of compound name column to equate automatic may then yield a .sdf which is not understood, e.g. by openbabel (version 3.0.0, April 2020).

The suggestion for this type of .sdf export by DW is to report the molecules names in the data's header / footer on one line, separated only by a blank space.

The archived .dwar equally contains cells with more than one multiple occurrence of the same PubChem number (e.g. cell #46 about PBCHM2982, PBCHM47354, and PBCHM40585).

The desideratum for cases like this one is to retain only one occurrence of each PubChem number per cell.

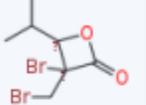
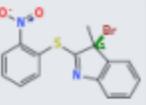
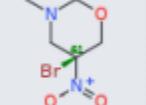
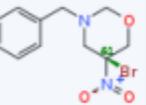
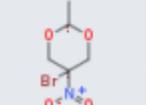
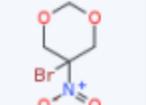
[1] https://github.com/IanAWatson/Lilly-Medchem-Rules/blob/master/test/example_molecules.smi, revision Apr 26, 2020

[2] E.g., <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4702940/>

File Attachments

1) [format_suggest.png](#), downloaded 1086 times

sorted_DW_deduplicate_structure.dwar

Table	Structure	Molecule Name
101		PBCHM556883
102		PBCHM94388
103		PBCHM10009242 PBCHM10009243
104		PBCHM202959 PBCHM202960
105		PBCHM201656
106		PBCHM40955
107		PBCHM1807
		PBCHM9990042

```

Terminal
=====
*** Open Babel Warning in ReadMolecule
WARNING: Problems reading a MDL file
Cannot read atom and bond count
Expected standard 6 character atom and bond count

102 molecules converted

Terminal
File Edit View Terminal Tabs Help

4 > <Molecule Name>
3 PBCHM94388
2
1 $$$$
4410 PBCHM10009242
1 PBCHM10009243
2 Actelion Java MolfileCreator 2.0
3
4 0 0 0 0 0 0 0 V3000
5 M V30 BEGIN CTAB

Terminal
File Edit View Terminal Tabs Help

3 M V30 END BOND
2 M V30 END CTAB
1 M END
4503 <Molecule Name>
1 PBCHM10009242
2 PBCHM10009243
3

```

- 2) [testinput.zip](#), downloaded 657 times
 3) [sorted_DW_deduplicate_structure.dwar.zip](#), downloaded 689 times