
Subject: Re: Exporting a descriptor as a Textfile
Posted by [nbehrnd](#) on Sat, 21 May 2022 16:48:02 GMT
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Christophe,

for a small set of molecules, I think I'm able to replicate your findings e.g., for the assignment and subsequent display of skelspheres as a string:

(observation with DW 5.5.0 for Linux, including the update by May 13th).

On the other hand (now specific to skelspheres); if these are like fingerprints e.g., openbabel offers,^[1] what are programs you intend to use which accept these as an input for further computation?

E.g., openbabel reports about DMF:

```
$ obabel -:"CN(C)C=O" -ofpt -xf FP2
> 5 bits set
00000000 00000000 00000000 00000000 00000000 00000000
00000000 00000000 00000000 00000000 00200000 00000000
00008000 00000000 00000000 00000000 00000000 00000000
00000000 00000000 00000000 00000400 00000000 00000000
00000000 00000000 00000000 00000000 00000000 00040001
00000000 00000000
1 molecule converted
```

or

```
$ obabel -:"CN(C)C=O" -ofpt -xs -xf FP2
>
0 6 1 7 1 6 <693>
0 7 1 6 <82>
0 8 2 6 <623>
0 8 2 6 1 7 <330>
0 8 2 6 1 7 1 6 <64>
1 molecule converted
```

Norwid

[1] https://open-babel.readthedocs.io/en/latest/FileFormats/Fingerprint_format.html

File Attachments

1) [example_str_skelspheres.png](#), downloaded 1609 times

molecules.dwar

File Edit Data Chemistry Database List Macro Help

Table	Structure	str_SkelSpheres
1		<i>[Illegible]</i>
2		<i>[Illegible]</i>
3		<i>[Illegible]</i>
4		<i>[Illegible]</i>
5		<i>[Illegible]</i>

Table Form View

170 of 502 MB Selected:1 Visible:5 Total:5

str_SkelSpheres

Column Name
str_SkelSpheres

Structure

2) [molecules.dwar](#), downloaded 636 times