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

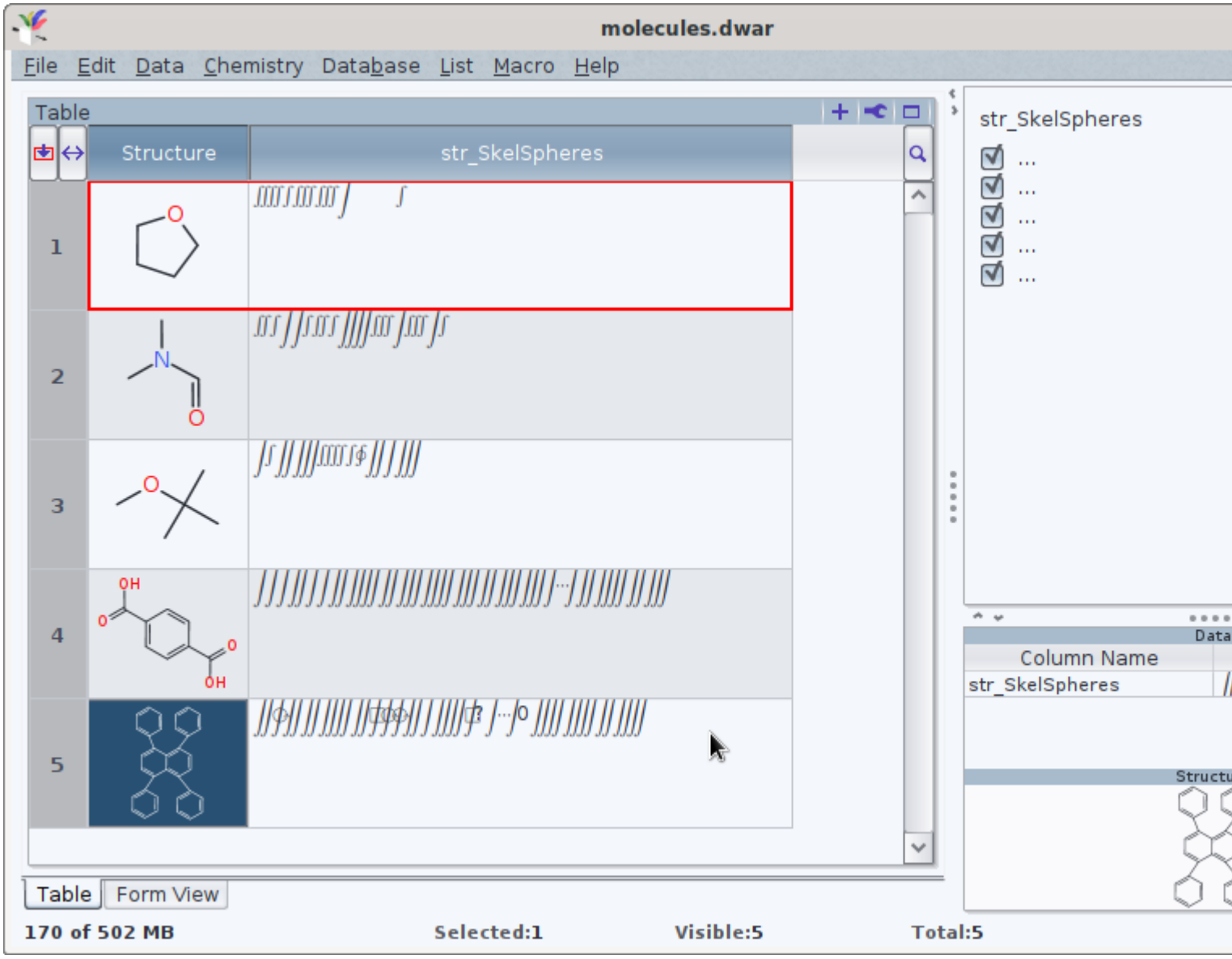
```
$ obabel -:"CN(C)C=O" -ofpt -xs -xf FP2
>
0 6 1 7 1 6 <693>
0 7 1 6 <82>
0 8 2 6 <623>
0 8 2 6 1 7 <330>
0 8 2 6 1 7 1 6 <64>
1 molecule converted
```

Norwid

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

File Attachments

1) example_str_skelspheres.png, downloaded 1952 times



2) molecules.dwar, downloaded 706 times