
Subject: Re: name vs score 2D plot

Posted by [nbehrnd](#) on Tue, 07 Mar 2023 14:52:35 GMT

[View Forum Message](#) <> [Reply to Message](#)

Hi sublimeuser,

is it possible for you to share a typical, yet not confidential .sdf presenting the problems to you? I speculate perhaps the problem correlates with the syntax in the input file.

In an instance of Linux Debian 12/bookworm with openbabel (vesion 3.1.1) I created two .sdf files where the «compound name» is the standard InChI key

```
``` shell
$ obabel -:"O" -:"CCOCC" -:"c1ccncc1" -h --gen3d --append "inchikey" -O testV2000.sdf
$ obabel -:"O" -:"CCOCC" -:"c1ccncc1" -h --gen3d --append "inchikey" -x3000 -O testV3000.sdf
```
```

This is to cover both the elder V2000 format, as well as the contemporary V3000 one DW prefers on file I/O as .sdf. The reading from the CLI was in pattern of

```
``` shell
$ datawarrior ./testV3000.sdf &
```
```

run without noticeable difficulty, nor the adjust the header "compound name" by "InChI key" - there was a prompt (automatic) update in the 2D and 3D plot on abscissa and ordinate.

The four tests run DataWarrior 5.5.0 in said Debian, either the one provided by a pristine installation with the installer fetched by 2022-05-18 (i.e., the state by 2021-04-03), or by subsequent application of the update fetched today (2023-03-07) about the state reached by 2024-02-24.

With regards,

Norwid

File Attachments

- 1) [testV2000.sdf](#), downloaded 80 times
 - 2) [testV3000.sdf](#), downloaded 82 times
 - 3) [testV2000.dwar](#), downloaded 87 times
-