
Subject: Structure No Column

Posted by [sbembenek18](#) on Thu, 24 Oct 2019 03:04:27 GMT

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

I am trying to understand what it is about my SDF file that cause Data Warrior to include a 'Structure No' column upon reading it. thanks.

Subject: Re: Structure No Column

Posted by [nbehrnd](#) on Thu, 24 Oct 2019 15:59:11 GMT

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

Is there a sdf minimal in size (i.e., less than 2MB) without confidential content you may attach here as an example triggering this in DataWarrior?

Subject: Re: Structure No Column

Posted by [sbembenek18](#) on Thu, 24 Oct 2019 17:50:17 GMT

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

Here's two examples.

File Attachments

- 1) [cats_mol_PP_rm_all_write_props.sdf](#), downloaded 434 times
 - 2) [cats_mol_PP_write_props_molecule_name.sdf](#), downloaded 433 times
-

Subject: Re: Structure No Column

Posted by [thomas](#) on Thu, 24 Oct 2019 19:25:46 GMT

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

I just checked the source code to answer. DataWarrior automatically generates this column as a unique row identifier, unless the molfiles in the sd-file contains names or unless another field with an obvious name provides such an identifier, e.g. "ID", "IDNUMBER", etc. If you don't need the column, you may delete it immediately after loading the sd-file.

Subject: Re: Structure No Column

Posted by [sbembenek18](#) on Fri, 25 Oct 2019 01:23:02 GMT

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

thanks
