Subject: Structure No Column
Posted by sbembenek18 on Thu, 24 Oct 2019 03:04:27 GMT
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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
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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
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Here's two examples.

File Attachments
1) cats_mol_PP_rm_all_write_props.sdf, downloaded 839 times
2) cats_mol_PP_write_props_molecule_name.sdf, downloaded 810 times

Subject: Re: Structure No Column
Posted by thomas on Thu, 24 Oct 2019 19:25:46 GMT
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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
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thanks