Subject: add empty rows

Posted by chemty on Fri, 11 May 2018 14:24:31 GMT

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Hi,

I have a question about adding empty rows. If I read in an sdf and add an empty row, I get no errors, but it doesn't show up. I reset all the filters, still no new empty row. If you look at the count of rows it shows it's been added. If I read in a smiles text file, I can add an empty row and add a new structure, no problem and it shows the new row. Is there something else to consider when adding rows to an sdf vs other files?

Thanks, Greg

Subject: Re: add empty rows

Posted by thomas on Fri, 11 May 2018 16:25:52 GMT

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Hi Greg,

I assume that your SD-File contains some data in addition to the chemical structure and that you get default 2D- and 3D-views after opening the SD-file, with some of that data associated to some axes. Since a new row won't have the information, it is not shown in these views. And because the concept is that all views show the same data, these empty rows are not visible in table and structure view either. In these cases a graphical view serves as implicit filter. If you close these views of put them behind the table or structure view, you should see all rows. An invisible view does not hide rows. You may also explicitly change the graphical views default behaviour to not influence row visibility of other views (Set Graphical View Options->Row Hiding->Hide Invisible Rows in Other Views).

Thomas