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Subject: SOM generation.

Posted by [timritchie](#) on Tue, 03 Feb 2015 13:58:39 GMT

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Hello,

I am trying to create a SOM using the SkelSpheres descriptor, which I calculated in DataWarrior. However in the SOM dialogue box, the structure descriptor is not listed in the parameters to select.

Am I doing something wrong?

Regards,

Tim Ritchie.

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Subject: Re: SOM generation.

Posted by [thomas](#) on Thu, 05 Feb 2015 21:55:04 GMT

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Hallo Tim,

I see two possible explanations:

- If you have a large file and the SkeletonSpheres calculation is still underway when opening the SOM dialog, the descriptor does not show up.

- More likely: If some rows don't have chemical structures and therefore also miss the descriptor, it won't show up either. To solve the problem you may sort the structure column by clicking on its header, then scroll the table to the very end, select all empty structures and delete them with Data->Delete Rows->Selected Rows. If you open the SOM dialog after that, you should see the SkeletonSpheres descriptor.

Best wishes,

Thomas

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