
Subject: Re: Can you disable SMILES conversion?
Posted by [zsolt](#) on Mon, 14 Dec 2020 23:32:07 GMT
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Thank you very much for the reply - this works, the processing is much faster indeed.

The only issue now is that when I try to set these plain SMILES strings to be on one of the axes of the 2D plot I get the error message "Column <column name> is neither a descriptor nor does it have a numerical variance" if I try to use it from a macro and it is missing from the options if I try to set it through the GUI. It makes sense not to be able to set a string as one of the axes however it seems to be possible for other string/plain text type columns - presumably because they are "descriptor"s. Is there a way for these plain-text-SMILES columns to be specified as an axis of the 2D and 3D plots?

Thanks,
Zsolt
