Subject: Re: Linux version bugs
Posted by nbehrnd on Mon, 24 Jan 2022 08:48:54 GMT
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Dear Thomas,

the problem exporting the .sdf was noticed (yet not reported) because it still was possible to assign SMILES to the structures then exported in a text file. After accessing the column in question (via awk), OpenBabel provided external regeneration of the .sdf.

Norwid