Subject: Re: SMILES Code
Posted by Anne on Thu, 21 Sep 2023 02:06:13 GMT
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:o :o :o Thank you so so much for your reply. I have sent the examples to you. Sorry that I spend some time to make this clear.

While I use “paste special” to transform the data from EXCEL, the SMILES code transform to each corresponding structure successfully without message.

While I try to add a whole new structure to the DataWarrior after the paste special step, countless messages will pop out. I need to correct my previous report. Regardless of the stereochemistry, the unexpected message will show. “CC(=O)C” also has the same outcome.

When I paste the “O[C@H]1[C@H](O)[C@@H](CO)OC=C1” to different conditions, different situations will show.

Please feel free to let me know any idea from you. I can try.