Subject: Re: SMILES Code Posted by thomas on Wed, 13 Sep 2023 15:53:05 GMT View Forum Message <> Reply to Message

I tried to reproduce the problem, but failed. When I paste the SMILES from your message I always got the proper molecule or substructure, depending on the context. I tried directly in the table view, in a structure filter (directly and after opening the editor). I also tried in the Chembl retrieval dialog in substructure and similarity modes. I also tried with the old V5.5.0 as well as with the current development version.

There must be a different reason. What is the source of the SMILES? May there be invisible characters in between? Can you help me to reproduce the error? Which OS do you use? I suggest to update to the dev version (go to DataWarrior download page, click on 'read and understood..., and find the update link in the small print).

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