Subject: Re: SMILES Code

Posted by Anne on Mon, 18 Sep 2023 08:55:50 GMT

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Thank you for your kind and prompt reply. The SMILES code is transformed via ChemDraw. I can also obtain the structure in DataWarrior via that SMILES code, but it seems the error message is unavoidable. I need to press "OK" to make the system accept the structure. However, there is no error message when I paste the SMILES code "C1CCCC1C2CCCC2", which corresponding to a structure without any stereochemistry information.

We install the DataWarrior on Win10, traditional Chinese version. Would this error caused by the conversion between double-byte and single-byte system?