Subject: Errors calculating flexophore-based similarity/activity cliff of certain molecules
Posted by user on Tue, 11 May 2021 07:35:12 GMT
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Flexophore-based similarity/activity cliff analysis of a dataset that contains non-standard SMILES of tetrazoles no longer works after upgrading to datawarrior 5.5.0 (used to work in datawarrior 5.2.1).

Error message I got:

Standardized SMILES of the same compounds didn't cause any errors in datawarrior 5.5.0.

When importing the SMILES strings from a CSV file it seems that the SMILES to structure conversion also gives weird bonds, which may cause this issue (manually pasting the SMILES into structure editor gives no errors). Other compounds may also have this issues since I got like hundards of error messages while working on a diverse dataset of over 7K molecules, but I have only confirmed on tetrazoles.

An example .csv file and the resulting problematic .dwar file that could reproduce the problem is attached for reference.

## File Attachments

1) error.csv, downloaded 558 times
2) error.dwar, downloaded 540 times
3) error.png, downloaded 894 times