Subject: tox predict folder

Posted by pc419714@ohio.edu on Tue, 16 Apr 2019 22:03:22 GMT

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I tried opening the files in the tox predict folder of data warrior but for some reason data warrior will not let me view the fragments. From my understanding these are the fragments that are used to calculate tumorgenicity, mutagenicity, and developmental effect. Is there any way to view these?

Subject: Re: tox predict folder

Posted by thomas on Wed, 17 Apr 2019 18:11:49 GMT

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For txt files DataWarrior needs a first line to contain TAB separated column names. The column that contains the encoded structure (called idcodes) must be named 'idcode' or it should end with ' [idcode]' for DataWarrior to show structure. dwar files, the native DataWarrior files' are much more flexible, but also much more complicated. Thus, keep/use the 'txt' extention and make sure that you have the key word 'idcode' in the first line and correct column.

**Thomas**