Subject: Re: Can you disable SMILES conversion?
Posted by thomas on Sat, 19 Dec 2020 11:36:08 GMT

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In this case the 'Smiles' column is a normal text column, for which DataWarrior keeps a sorted list of available categories unless the number of different text entries exceeds 65536. As long as the number of distinct smiles values (categories) stays below that value, the column is considered to contain categories and can be assigned to an axis. Categories have a natural or user-selected order and, therefore, individual smiles can be assigned a numerical value (its position in the category list), which is used to position it on the axis. If the number of distinct values in a column is larger than 65536, then DataWarrior doesn't maintain a category list anymore. Then it cannot assign numerical values to individual smiles to position them on an axis. For efficiency reasons there must be a limit.