Subject: Re: Molecule style & color
Posted by thomas on Wed, 08 Jul 2020 20:09:47 GMT
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Hallo Paul,

with version 5.0.0 DataWarrior switched from JMol as 3D-molecule-viewer to FXMolViewer.
This involved many changes, e.g. instead of having a grid view 0f 3x3 conformers, all
conformers are now superpositioned in one view. A slider allows to separate the conformers.
The new viewer is much more flexible, has lots of features, which DataWarrior will use in
future updates and is based on the same cheminformatics library that DataWarrior itself uses,
this was an overdue and obvious change. However, you are right that the default molecule mode
changed from ball&sticks to sticks only, which seemed more appropriate for superpositioned
conformers. To better distinguish superposed conformers they have different colors.
Nevertheless,
hetero atoms are shown in their native color (N=blue, O=red, etc).

Currently, DataWarrior does not use Settings of any kind. Would it help in your opinion, if you
could
change all molecules to ball&sticks with a new popup menu item?

Thomas