Subject: Molecule style & color
Posted by Paul on Wed, 08 Jul 2020 18:39:16 GMT
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Hello,

In version 5.02.01, the molecule style and color defaults for conformers have changed. How do I change the defaults back to ball and stick and color by atomic number?

Thanks,

Paul

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

Subject: Re: Molecule style & color
Posted by nbehrnd on Wed, 08 Jul 2020 22:42:28 GMT
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Hello Paul,

if the window including the 3D representation is large enough, you may mark a bond or an atom of the molecule displayed (left mouse click, turning the selected red) then

followed by a right click. This action opens a new menu with adjustable entries about molecule style (including «Ball And Sticks») and molecule colour (with «By atomic No»).

This works equally well for the representation of single molecules (as shown in the series of 01.png till 03.png, attached below), as well as for the simultaneous display of conformers (04.png and 05.png). This menu may be closed by «Esc».

Norwid

File Attachments
1) 01.png, downloaded 267 times
2) 02.png, downloaded 571 times
3) 03.png, downloaded 290 times
4) 04.png, downloaded 272 times
5) 05.png, downloaded 281 times

Subject: Re: Molecule style & color
Posted by Paul on Thu, 09 Jul 2020 00:59:32 GMT
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Thanks for the information (and the program in general).

Carbon and hydrogen atoms are displayed in the same color - 7fffd4. Nitrogen and oxygen atoms are their usual colors (blue and red).

It would be somewhat of an improvement if carbon were grey, dark grey or black. Or different from hydrogen.

I am able to use the right click menu to change molecule style and colors, on a per molecule basis.

When working with files of thousands of different molecules, the right click option is impractical.

Sticks versus balls and sticks is purely cosmetic, so I can live with just sticks, and might actually appreciate the benefits of superimposition of conformers.

I need to be able to differentiate carbon from hydrogen atoms, though.

Again, thanks!

Paul

Subject: Re: Molecule style & color
Posted by nbehrnd on Thu, 09 Jul 2020 07:57:52 GMT
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Hello Paul,

a quick work-around could employ the platform independent Jmol.(1) It is possible to save all of the conformers generated in one .sdf file in common -- just take care that the export retains the 3D coordinates (which is not the default).

In Jmol running, the entry File -> Console opens the programs' own little terminal. Then indicate Jmol the .sdf to read; it will recognize that the .sdf contains multiple models, but by default will display only the first one. This is the chance to disable the display of double / aromatic / triple bonds with more than one line (by the second command), to adjust the diameter of the sticks and balls (third command) and eventually display all models (here: all superimposed conformers) at once by the instruction of model 0.

The scene may be exported like below.

The interaction with Jmol may be scripted (e.g., 2,3,4) thus you may reuse instructions more than once. If the color of an atom type does not fit your needs, for example, you could alter the representation by

select hydrogen
color gray

for all models load at once. You may return to the default color scheme by

select all
color cpk

Norwid

1) http://wiki.jmol.org/index.php/Main_Page
2) https://chemapps.stolaf.edu/jmol/docs/
3) https://earth.callutheran.edu/Academic_Programs/Departments/BioDev/omm/jsmol/scripting/molmast.htm#V
4) Hanson, J.Appl.Cryst.(2010).43, 12501260, doi: 10.1107/S0021889810030256

File Attachments

1) console.png, downloaded 625 times
2) example.png, downloaded 636 times

3) liquid_crystal.dwar, downloaded 301 times
4) DW_conformer_generation.png, downloaded 274 times
5) conformers.sdf, downloaded 262 times

Subject: Re: Molecule style & color
Posted by Paul on Thu, 09 Jul 2020 16:52:57 GMT
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Nice!

Thanks for the help.

I will need to explore these options.

Best Regards,

Paul

Subject: Re: Molecule style & color
Posted by thomas on Fri, 10 Jul 2020 10:58:04 GMT
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Dear Paul,

I updated the behaviour. Hydrogen atoms of molecules, which are shown in a custom color, are now painted in an intermediate color:

Thomas

File Attachments
1) t.png, downloaded 616 times

Subject: Re: Molecule style & color
Posted by Paul on Mon, 13 Jul 2020 13:14:37 GMT
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That works good, Thomas.

Now I can benefit from conformer superposition and recognize methyl branches.

Thanks,

Paul