Subject: manually highlight atom/substructure in structure editor and structrue cell
Posted by Hong on Mon, 08 Jan 2024 03:19:21 GMT
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The functionality seems to be included in datawarrior because atoms were hilighted when do a substructure filtering. Is it possible to add a color function for manually highlight in structral editor and structral cell in the Table view?

Subject: Re: manually highlight atom/substructure in structure editor and structrue cell
Posted by thomas on Mon, 08 Jan 2024 09:50:39 GMT
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Currently, DataWarrior has two mechanisms for adding color to atoms:
- automatic by current structure filter settings or by similarity to the current reference row. This can be changed in the table header popup menu: "Highlight Structure By..."
- explicitly by a hidden column that defines atom colors for an associated structure column. An example would be the pKa reference file. Currently, there is no way to easily edit atom color by the user.

One could think of extending both coloring mechanisms for users to be more useful, e.g. let users provide a list of molecules or substructures that cause automatic coloring. One could also use substructure background highlighting. Or, as you propose, one could add an option in the editor to add color to individual atoms and store these colors inside the hidden column. Your question implies that you would like to edit atom colors individually for every structure, right?

Subject: Re: manually highlight atom/substructure in structure editor and structrue cell
Posted by Hong on Mon, 08 Jan 2024 12:14:36 GMT
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Hi Thomas,
Thansk very much for your timely reply.
Yes, I wanted to edit atom colors individually for every structure. e.g. I want to highlight sites of metabolite of some CYP inhibitors.
I noticed the pKa reference file and found some lines contain "red:0" "blue:1". I guessed it might be the color and innner atom index but had no idea to do it in datawarrior interface. Making hidden color column and atom index visible to the user might make it possible for the user to edit atom colors individually.
Thanks again for your time and again for your contributiing to open soource tool.