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Subject: Re: manually highlight atom/substructure in structure editor and structure cell

Posted by [Hong](#) on Mon, 08 Jan 2024 12:14:36 GMT

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Hi Thomas,

Thank 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 inner 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 contributing to open source tool.

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