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.