Subject: Re: Evolutionary algorithm

Posted by thomas on Tue, 12 Feb 2019 17:40:50 GMT

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When you define the first generation of molecules, then you may double click any of them to open the structure in the structure editor. Use the lasso tool and select the scaffold, which should not be touched. When selected, all scaffold atoms and bonds should be drawn in red. Then close the editor. In the list of first generation molecules, the unmutable scaffolds should still be drawn in red. When starting the evolution, these atoms and bonds won't be changed in any way. I just checked that this is still working. See example image...

File Attachments

1) elib.png, downloaded 596 times