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Subject: Re: fragments

Posted by [pc419714@ohio.edu](mailto:pc419714@ohio.edu) on Tue, 16 Apr 2019 20:56:14 GMT

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This is great! Thanks! One idea my boss had was to modify the code so that it calculated the drug score each generation and picked the best ones. I might try to modify the source code to try this but the way it is set up, if you select compounds with a high drug score to begin with, it generates compounds with high drug scores. We ended up doing 2 evolutions.

This is very helpful knowing more details about the fragments.

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