
Subject: Re: fragments

Posted by pc419714@ohio.edu on Tue, 16 Apr 2019 20:56:14 GMT

[View Forum Message](#) <> [Reply to Message](#)

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.
