Subject: drug score/evolutionary algorithm
Posted by pc419714@ohio.edu on Thu, 04 Apr 2019 18:14:15 GMT
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Hello Thomas,

The lab I work in is wondering why Data Warrior was programmed to only allow a certain number of compounds to survive each generation. For instance, if I set the properties in the evolutionary algorithm so that there are 400 generations, 4096 compounds per generation, and 32 surviving each generation, we end up with 12800 compounds surviving. From my understanding, the best compounds each generation have the best drug scores. We have 400 generations, but wouldn't generation 400 have the best compounds? So, why not only have compounds from generation 400 survive because previous generations would have lower drug scores? I would think if you did something like this, the compounds would all be pretty similar to one another and perhaps keeping 32 from each generation would allow for more diversity. Would the compounds from generation 1 be less fit than generation 400? What were the weights for the parameters you used to calculate the drug score?

Thanks! We will be sure to cite you. This is wonderful software.

Patrick Chirdon