
Subject: Re: Evolutionary algorithm

Posted by [thomas](#) on Sun, 10 May 2020 13:32:37 GMT

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not yet, but we are currently updating the flexophore algorithm. Providing one-conformer flexophore similarity is a natural next step. You may look into PheSA similarity as fitness criterion for the evolutionary library. PheSA (pharmacophore enhanced shape alignment) is not documented yet and still evolving, but the newest unofficial DataWarrior update (openmolecules.org/datawarrior/dw521win.zip & [dw521x.zip](http://openmolecules.org/datawarrior/dw521x.zip) for Windows and Linux/Mac, respectively) seems to work quite well. For PheSA-fitness you supply a ligand in its binding conformation and the fitness function give a high score if at least one candidate conformer may superpose nicely with the binding ligand conformer considering both: shape and pharmacophore features. The zip file contains just the DataWarrior.exe (datawarrior.jar for Linux/Mac) to replace the official 521 version. If you update this way, note that the flexophore is also updated, but not final yet. Thus, for using the flexophore, I recommend using the official 521 version.
