Subject: Re: Macro for evolutionary library (EL) in Datwarrior (DW)
Posted by nbehrnd on Thu, 08 Sep 2022 18:15:57 GMT
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Dear Jon,

the safest approach is to run the installer and the update A for version A. And if you want to check version B, to 1) deinstall DW, 2) run the installer, and 3) the updater for version B). This is by precaution because I do not know if updater A and B contain the same libraries by name the updated libraries of updater A may simply exchanged by those of updater B (like different tires on a car), .or. if they introduce changes in the other components of DW.

As for external literature references of evolutionary libraries .and. DataWarrior, my answer is no, I do not have a good i.e., tutorial-like literature reference at hand. Ningsih et al.[1] describe they used it, however address those who already are in the know:

(loc. cit. p. 18)

[1] Ningsih, E.G., Hidayat, M.F., Tambunan, U.S.F. (2019). Fragment-Based Drug Design to Discover Novel Inhibitor of Dipeptidyl Peptidase-4 (DPP-4) as a Potential Drug for Type 2 Diabetes Therapy. In: Rojas, I., Valenzuela, O., Rojas, F., Ortuño, F. (eds) Bioinformatics and Biomedical Engineering. IWBBIO 2019. Lecture Notes in Computer Science(), vol 11465. Springer, Cham. https://doi.org/10.1007/978-3-030-17938-0_2 pages 14–24 (paywall).

File Attachments

1) Ningsih2019.png, downloaded 1529 times

hydrogen bonds formed in the molecular interaction.

Fragment growing was conducted by utilizing DataWarrior software to create the evolutionary library which restricted to the FragFp descriptor, Lipinski's Rule of Five, Veber rules, drug-likeness above than zero and toxicity properties. Potential fragments were grown based on the Lipinski's Rule of Five (RO5) and Veber rules such as molecular weight <500 Da, rotatable bonds ≤ 10, TPSA <140 $Å^2$, and logP between −0.5 and 5.6, number of hydrogen donor <5, and number of hydrogen acceptor <10 [23]. At the end fragment growing process, around 62,392 generated ligands were stored in MDB format for the molecular docking simulation.

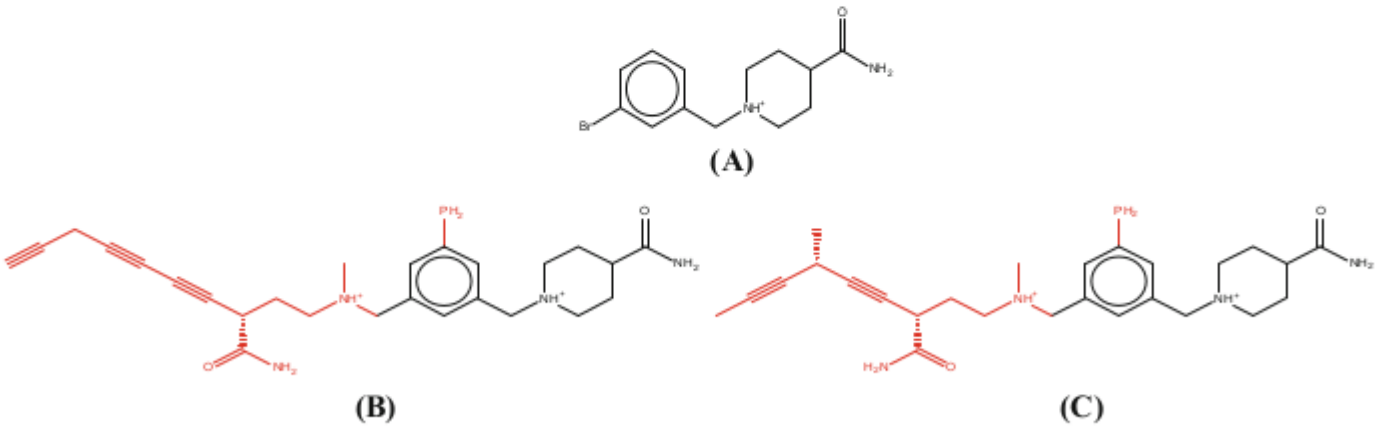

Fig. 2. Structure molecules of 1-[(3-bromophenyl) methyl] piperidine-4-carboxamide (A) along with fragment growing result, FGR-2 (B) and FGR-3 (C).