

Electronic Supplementary Information

Modeling of the binding of Octopamine and dopamine in insect monoamine transporters reveals structural and electrostatic differences.

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Supplementary Figures

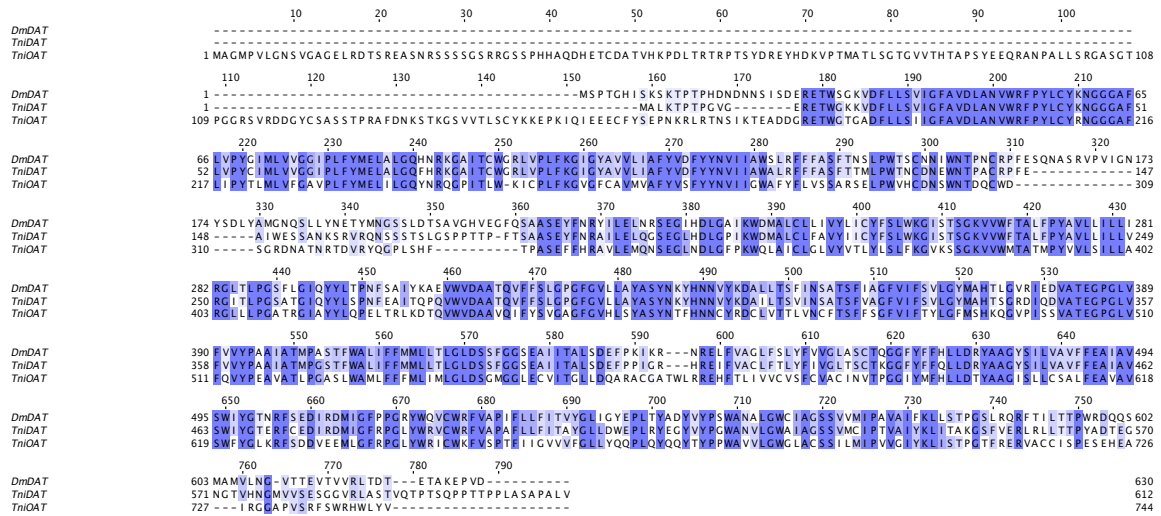


Figure S1: Alignment of amino acid sequences of Dopamine Transporter (DAT) of *Drosophila melanogaster* (Dm) and *Trichoplusia ni* (Tni) and Octopamine Transporter of *T. ni* (TniOAT). In blue boxes the amino acid identity is observed; dark blue represents 100% of residue conservation.

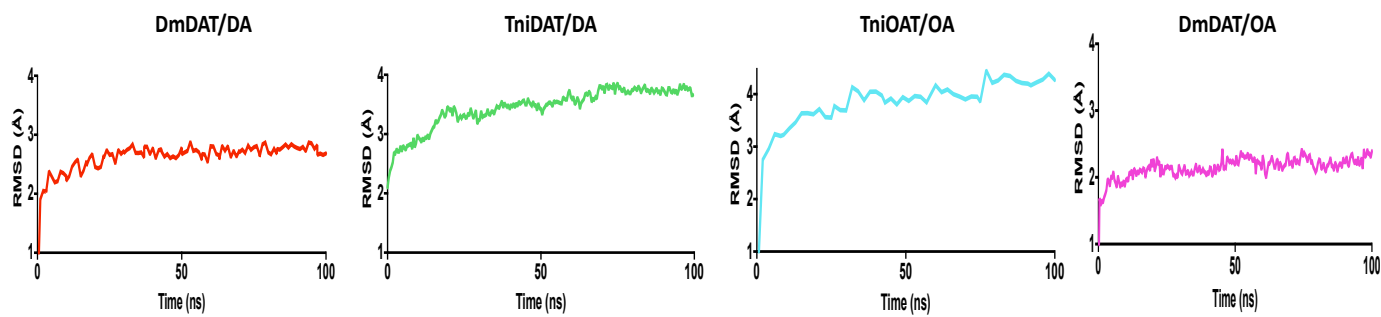


Figure S2: Molecular dynamics simulation time vs. root mean-square deviation values for all complexes simulated (DA in DAT of Dm:red and Tni:green; OA in TniOAT:cyan and DmDAT:purple)

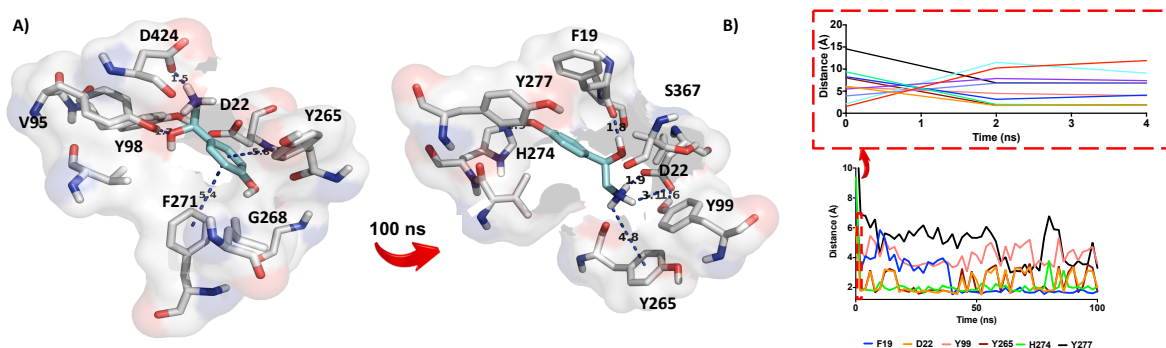


Figure S3: Octopamine exhibits a change respect to the initial conformation into the binding cavity (180°) A) octopamine inside the binding cavity of TniOAT at 0 and 100 ns. B) Representation of Distance vs. Time of simulation. The inset shows the specific time were the ligand change the orientation in the binding cavity.