

Allosteric Modulation of Human Dopamine Transporter Activity under Conditions Promoting its Dimerization

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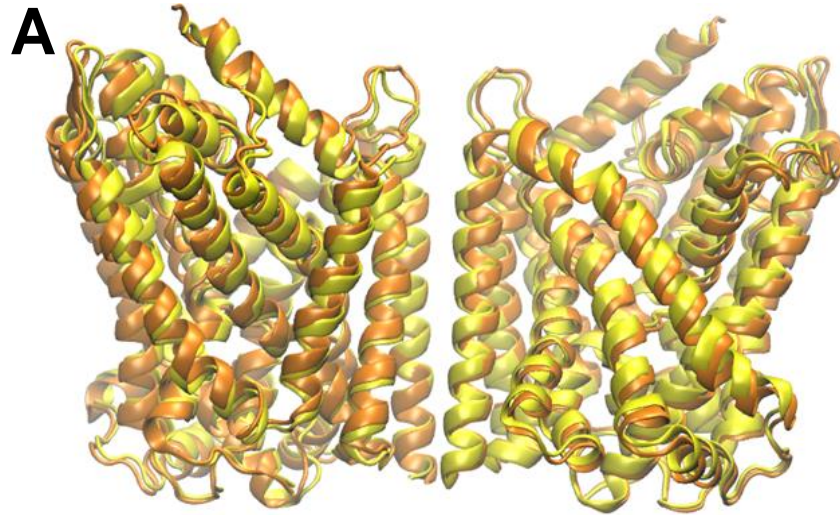
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Running title: *Human dopamine transporter dimerization*

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Supplementary Figures

Computed & X-ray structure for OFo LeuT dimer



Computed models for OFo & IFo LeuT dimers

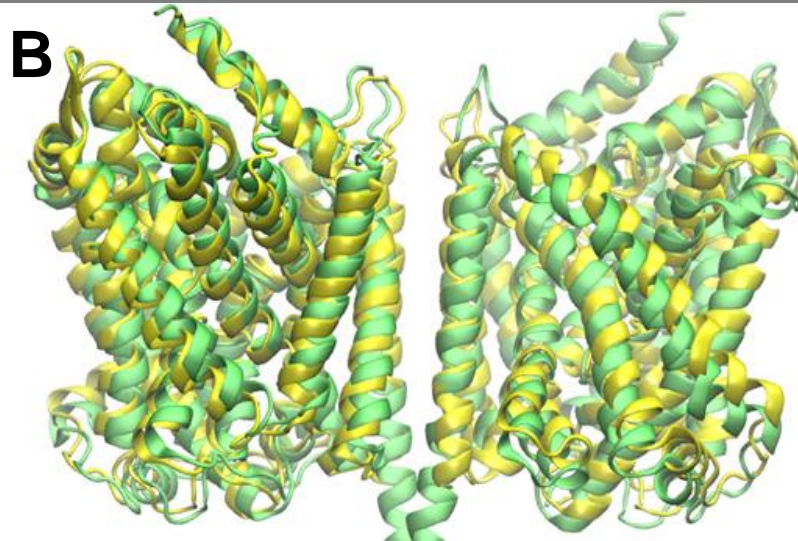


Figure S1: The computed LeuT dimer in different conformation states. **(A)** Comparison of the computed OFo LeuT dimer structure (*yellow*) with that structurally resolved (*orange*) (PDB: 3TT1). **(B)** Alignment of the computed OFo LeuT dimer (*yellow*) with the computed IFo LeuT dimer (*green*).

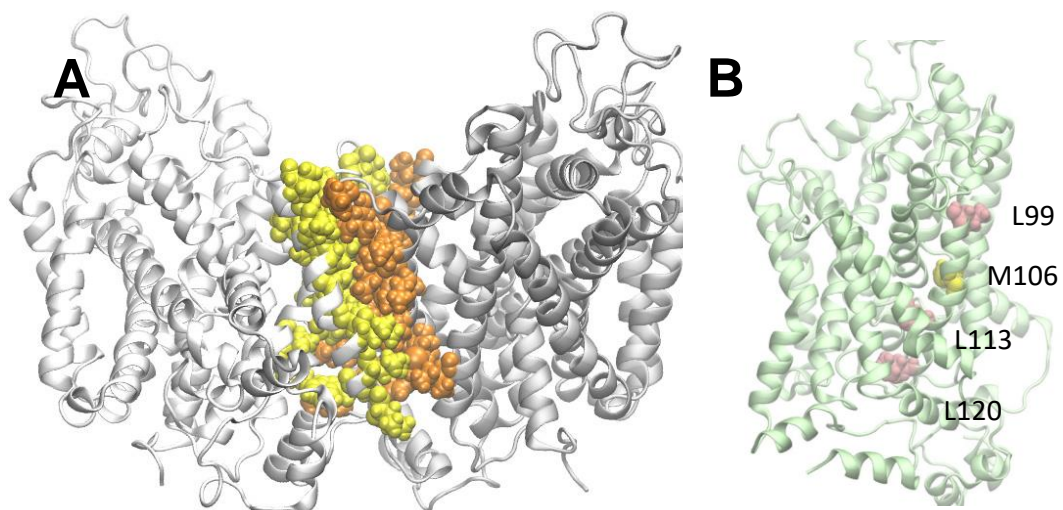


Figure S2: Large hydrophobic patch at the interface of the two subunits in the hDAT dimer. (A) Hydrophobic interfacial contact colored differently (*yellow* and *orange* represent hydrophobic residues from different subunits); (B) The predicted Leucine zipper (L99, M106, L113 and L120) (1) is not in direct contact. Instead one residue shift: V100, V107 and P112 contribute to direct interfacial interactions.