Electronic Supplementary Information for PCCP Article: Unveiling the Binding Mechanism of Orexin 2 Receptor Antagonists with Computational Chemistry

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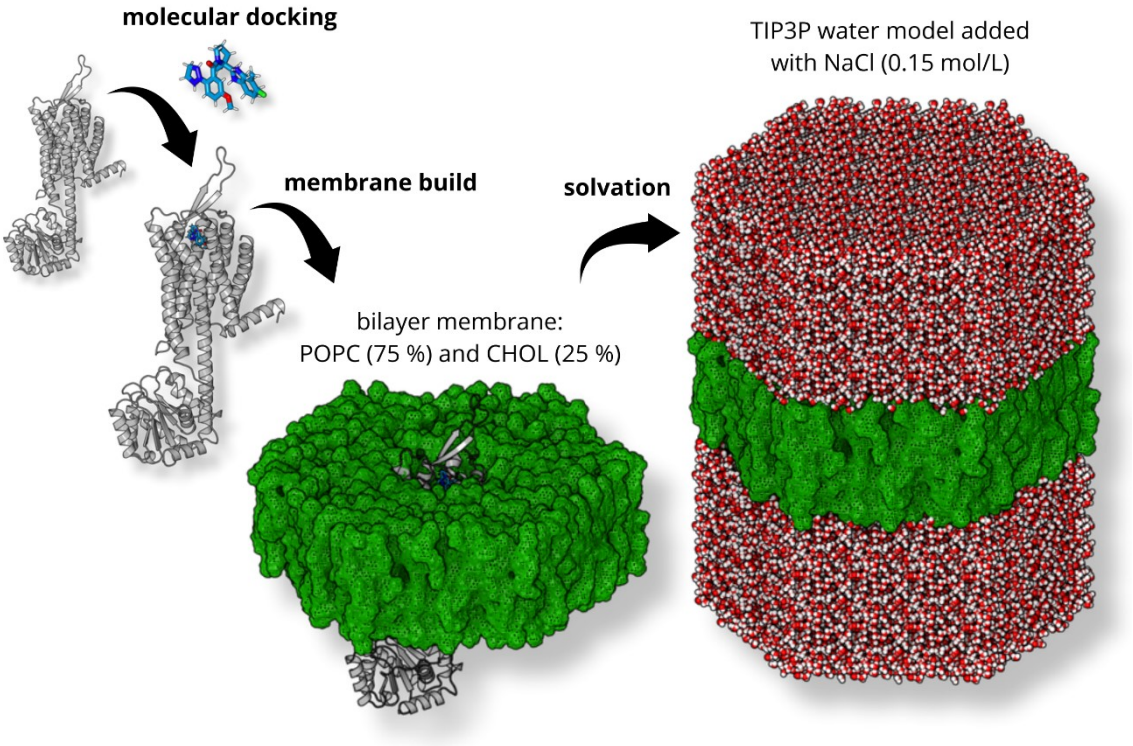

Fig. S1: Overall computational workflow. From molecular docking, insertion of the complexes into a lipid bilayer, ionic neutralization, and system solvation. The final panel depicts the complete simulation setup, with the receptor-ligand complex embedded in the membrane.