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Periplasmic Vestibule Determines the Ligand Selectivity in *E.Coli* AMTB UGUR AKGUN, SHAHRAM KHADEMI, University of Iowa — The transport of ammonia, fundamental to the nitrogen metabolism in all domains of life, is carried out by the Rh/Amt/MEP membrane protein superfamily. The first structure of this family, AmtB from *E.Coli* shows a pathway for ammonia that includes two vestibules connected by a long and narrow hydrophobic lumen. The accepted mechanism for AmtB is to recruit NH_4^+ and conduct neutral $NH_3$by deprotonation of NH_4^+ at the end of periplasmic vestibule. Here we report from various MD simulations performed using a model of trimeric AmtB embedded into POPE lipid bilayer to determine the mechanism of ligands selectivity and conduction in the ammonia channels. Our total more than 500ns simulations reveal that the AmtB periplasmic vestibule prefers NH_4^+ over NH_3 and CO_2. And the rate of ammonia conduction is regulated by the motion of the phenyl rings at the bottom of the vestibule. We also report that the conserved D160 is essential for ligand conduction by stabilizing the NH_4^+ at the recruitment site through charge interactions. Our simulations also suggest NH_4^+ most likely releases its proton to the bulk of water as it enters to the hydrophobic lumen.

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