

Supplemental Material

Allosteric and transport modulation of human concentrative nucleoside transporter 3 at the atomic scale

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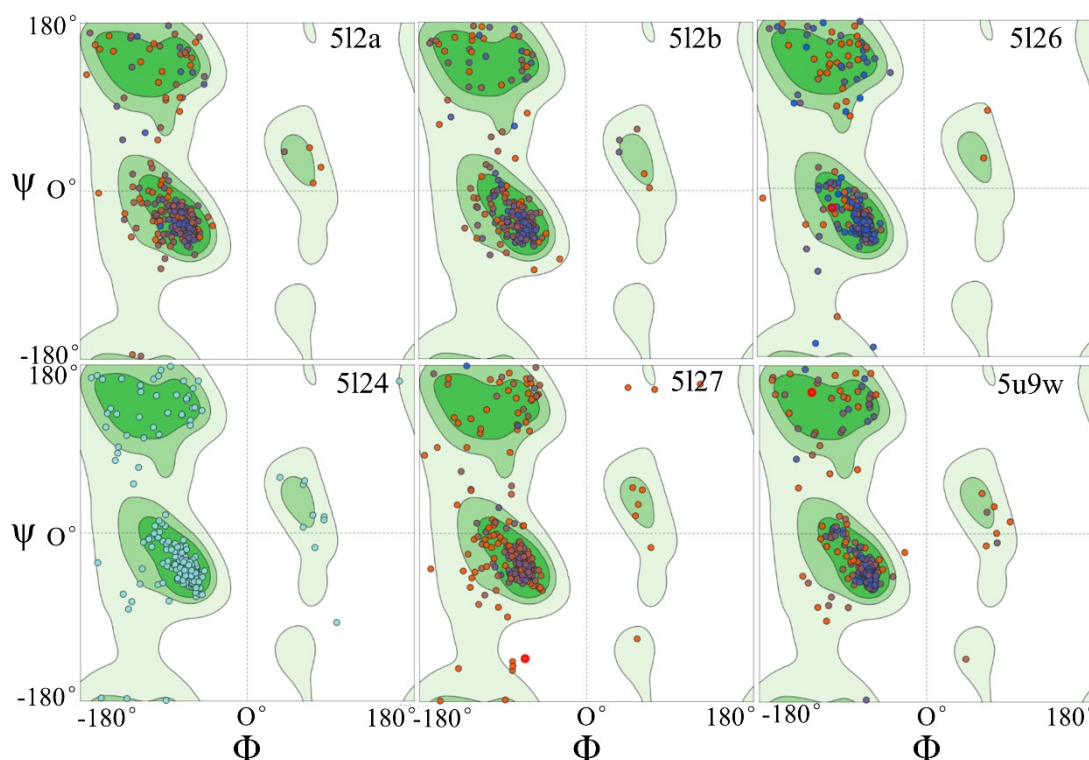


Figure S1 Ramachandran plots of CNT_{NW} model. Modelling quality from high to low is 5L26, 5L24, 5L2b, 5U9W, 5L2A and 5L27, with Q values of -3.09, -3.98, -4.39, -4.51, -5.10 and -7.09, respectively.

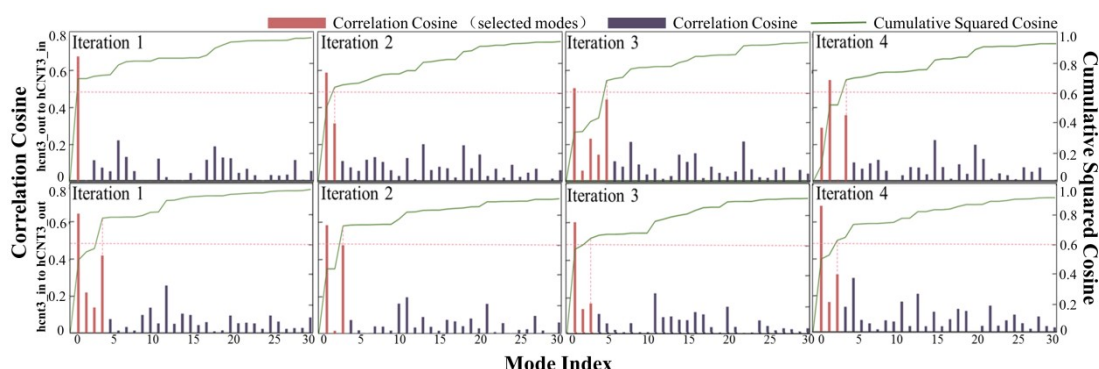


Figure S2 Correlation cosine between instantaneous distance vector and eigenmodes. Results are illustrated for aANM at the first 4 iterations, where the collection of intermediate conformations respectively starts with the outward-facing (i.e., hCNT3_out, the top 4 panels) and inward-fac structures (i.e., hCNT3_in, the bottom 4 panels) and approaches each other.

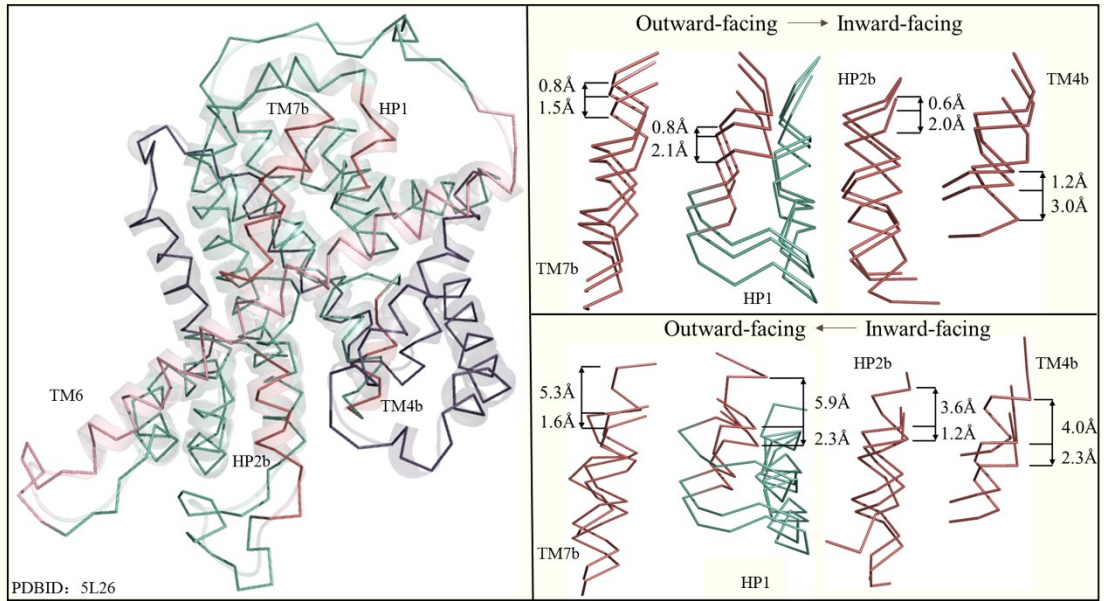


Figure S3 The offset distance of nucleoside transport channel during the transition from hCNT3_out and hCNT3_in to hCNT3_mid