Computational study for the unbinding routes of β-N-Acetyl-D-hexosaminidase inhibitor: insight from steered molecular dynamics simulations

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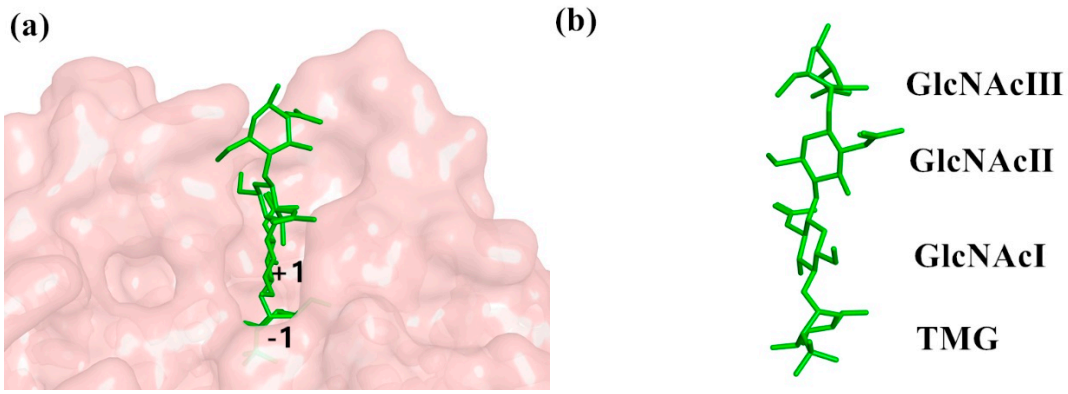


Figure S1. (a) The binding pocket of O*f*Hex1. (b) The structure of TMG-chitotriomycin.

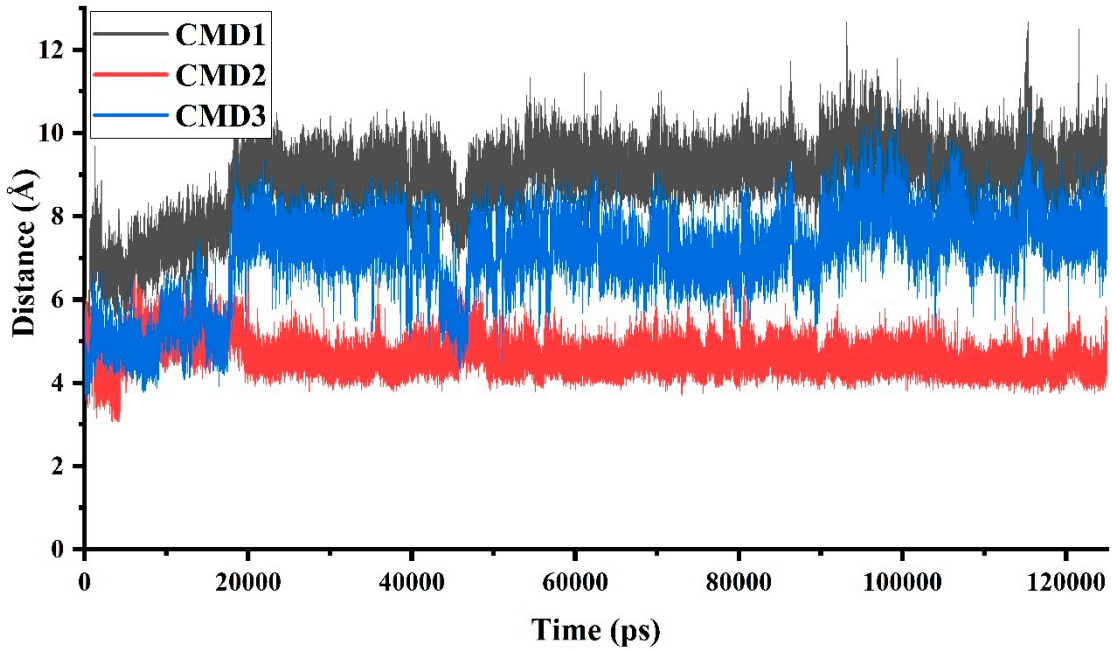


Figure S2. The distance between O4 atom of the ligand and NE1 atom of the receptor versus time. CMD1 in black, CMD2 in red, CMD3 in blue.

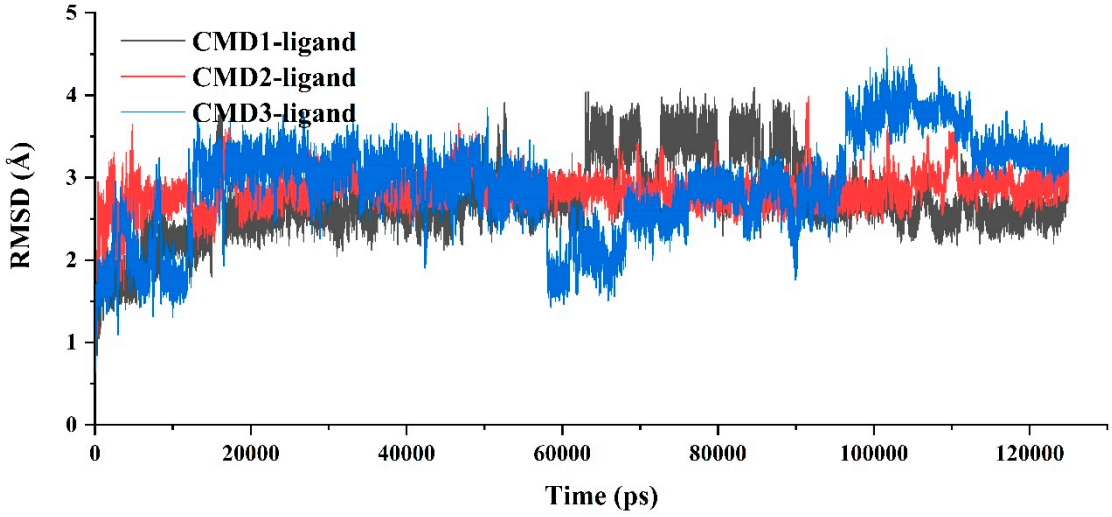


Figure S3. Root-mean-square deviation (RMSD) variation of ligand with respect to simulation time. CMD1 in black, CMD2 in red, CMD3 in blue.

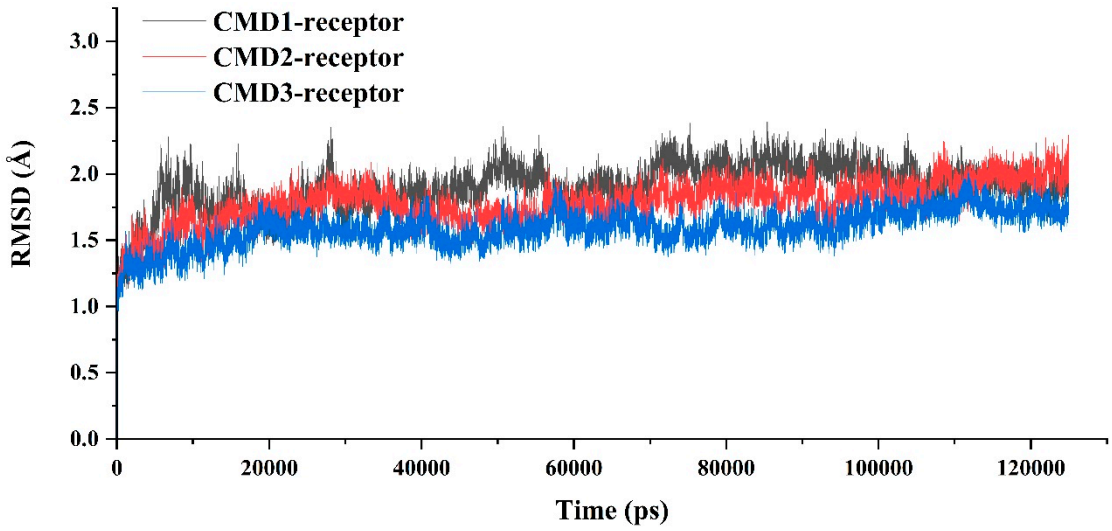


Figure S4. Root-mean-square deviation (RMSD) variation of receptor with respect to simulation time. CMD1 in black, CMD2 in red, CMD3 in blue.

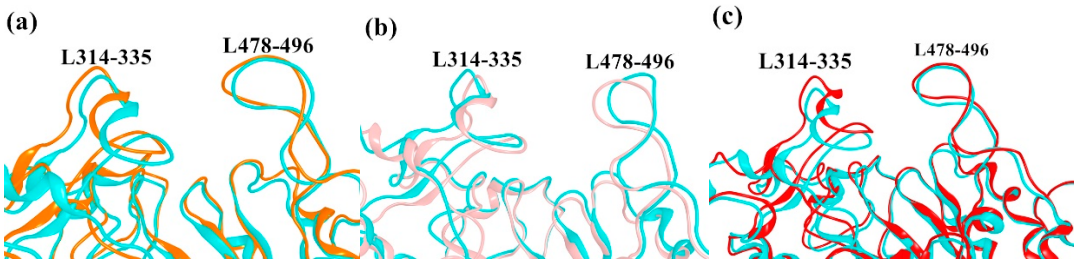
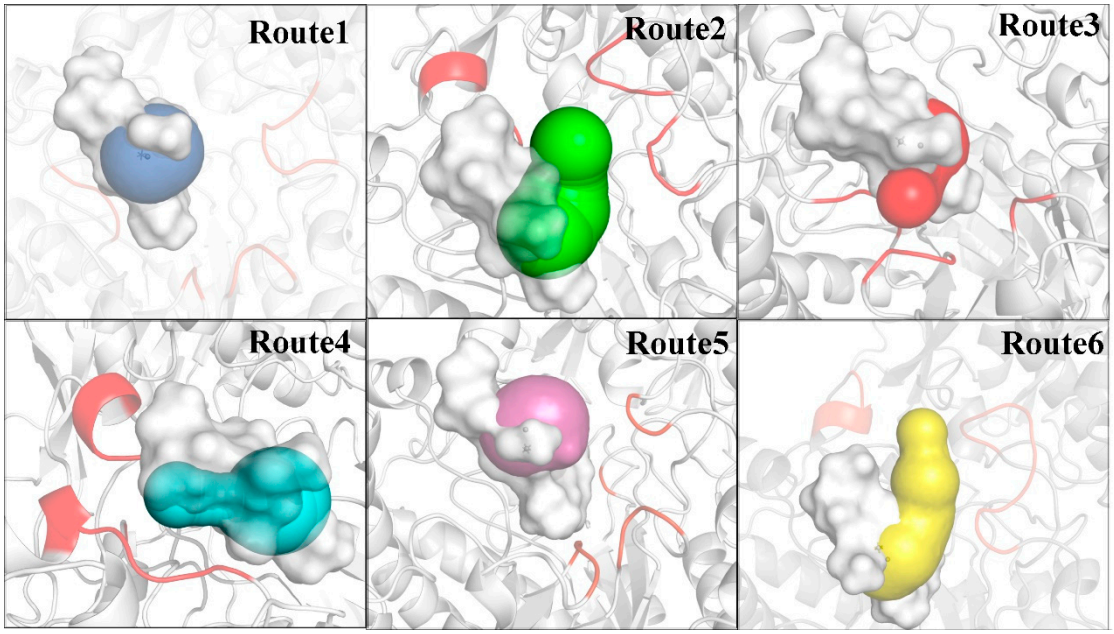


Figure S5. Structure comparison of two loops for the conversional MDs (a) CMD1 (yellow), (b) CMD2 (pink) and (c) CMD3 (red) with the crystal structure (blue).



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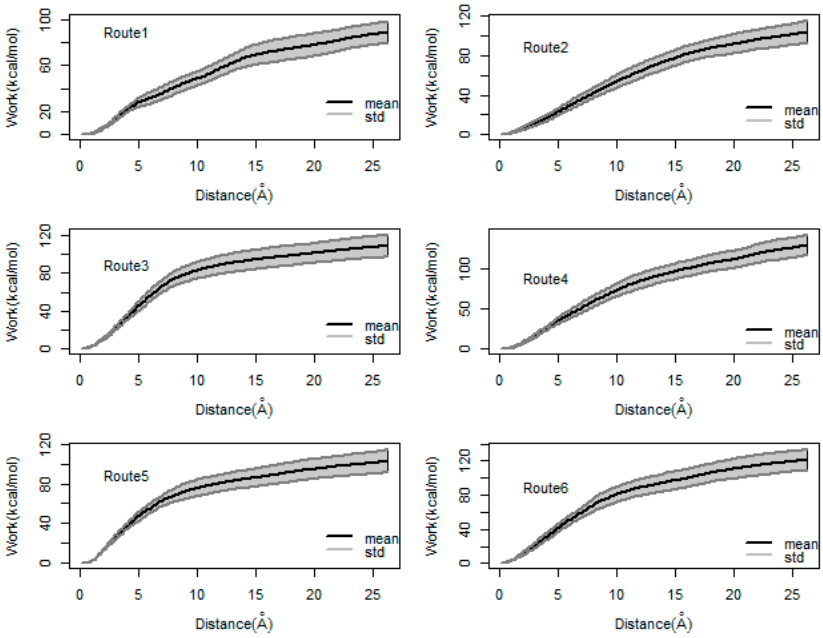

Figure S7. The average work versus the distance of ligand dissociation from the receptor