

Supplementary Materials

Molecular Dynamic Study on The Effect of N1 Neuraminidase Double Mutant G147R/H275Y to Oseltamivir Susceptibility

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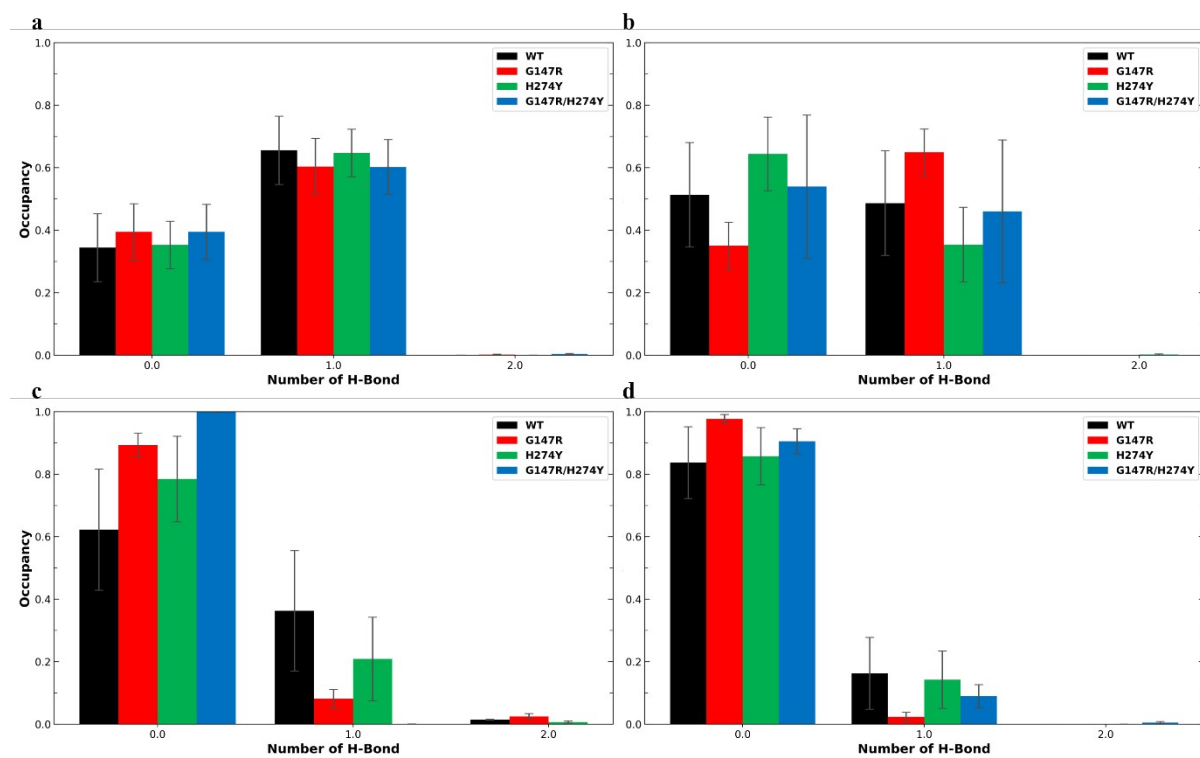


Figure S1. Hydrogen bonds occupancy formed by E119 (a), R152 (b), E227 (c), and E277 (d). The error bars indicated the standard error mean of replicates.

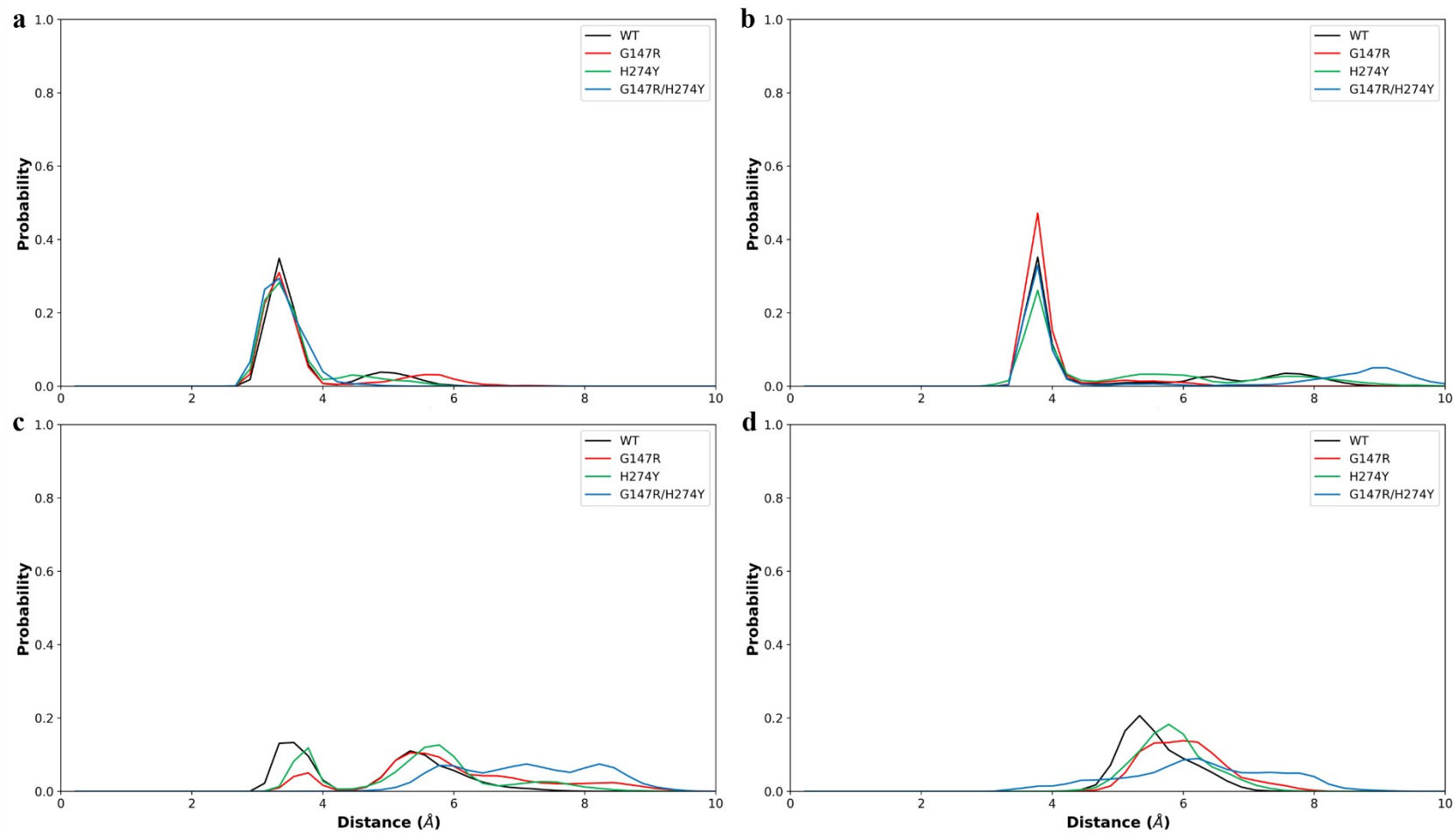


Figure S2. Normalized probability of the distance between N2 atom of OST with C-carboxyl of E119 (a), O3 atom of OST with C-guanidine of R152 (b), N2 atom of OST with C-carboxyl of E227 (c), and N2 atom of OST with C-carboxyl of E277 (d).

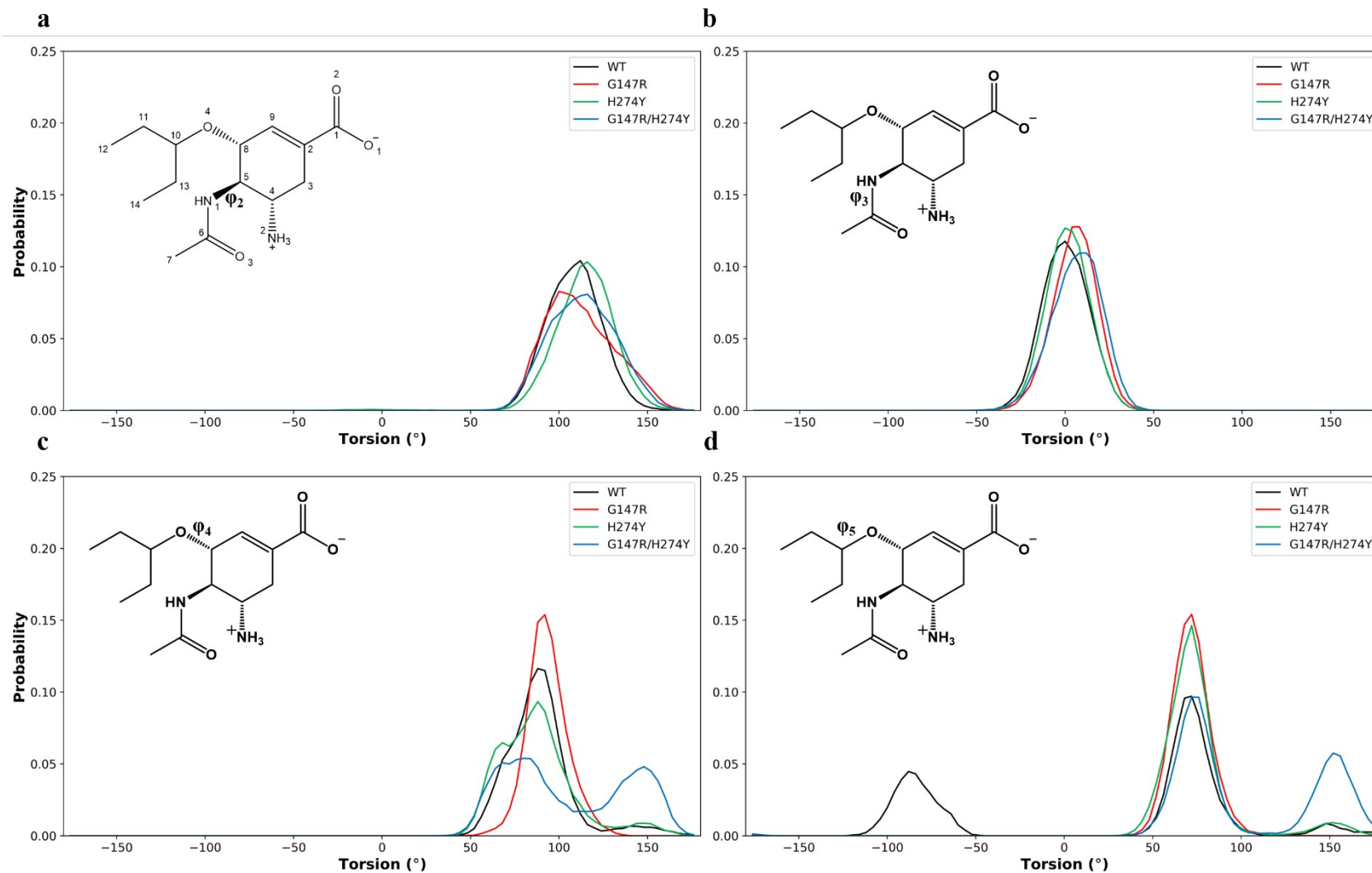


Figure S3. Normalized probability of the dihedral angle of φ_4 connecting pentoxyl moiety to cyclohexene (a), φ_5 connecting pentyl moiety to ether (b), φ_2 connection amide moiety to cyclohexene (c), φ_3 connecting acetyl moiety to amine moiety (d).

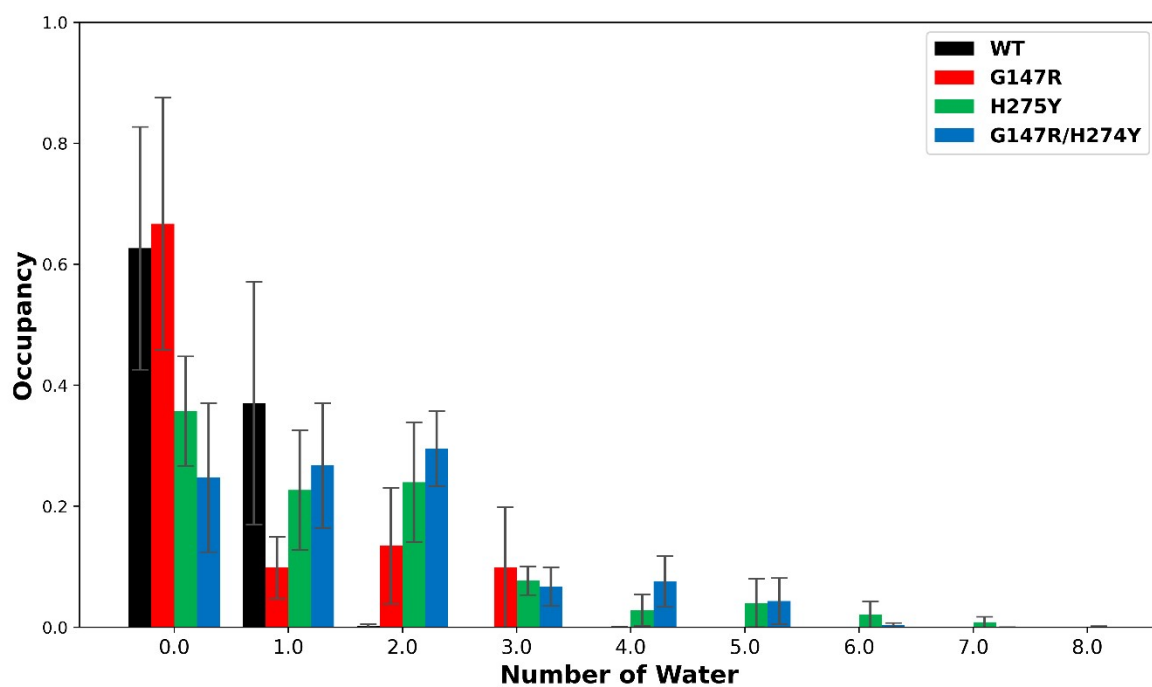


Figure S4. Normalized probability of water found near E276. Error bars indicated standard error mean of replicates.