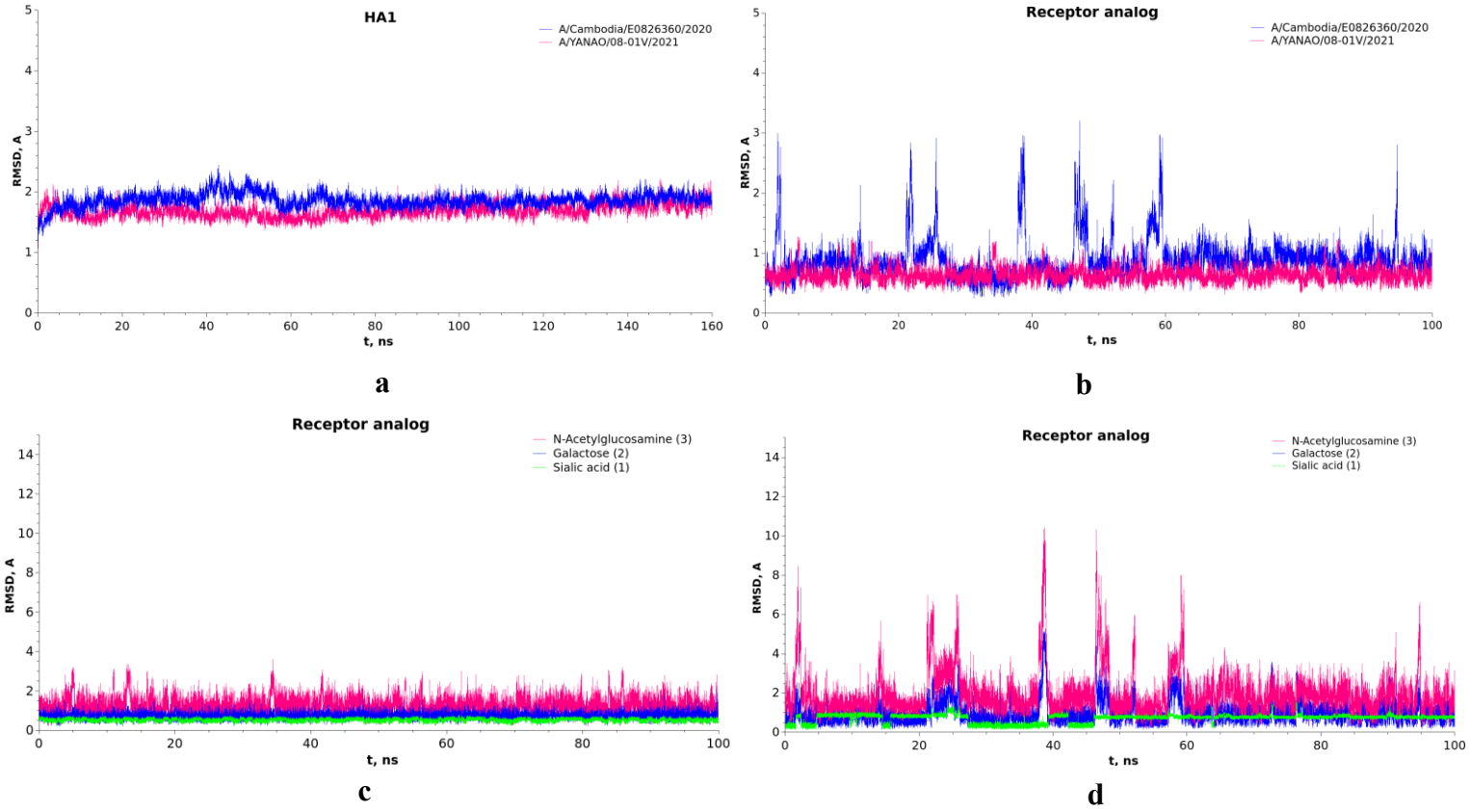
Figure S1: Time dependencies of atoms root mean square deviation



Root mean square deviations (a) of HA1 subunit bound to the receptor analog after the full simulation start; (b) of receptor analog after the equilibration process; per residue for the receptor analog with superimposing the sialic acid relatively to the first frame for the complexes with HAs of (c) A/ YANAO/08-01V/2021; (d) A/Cambodia/e0826360/2020.

Generally, non-close to the crystallographic pose conformations of the receptor analog in complex with HA of A/Cambodia/e0826360/2020 are associated with cooperative changes in glycosidic torsion angles and the exposure of the N-Acetylglucosamine part of the molecule to solvent (Figure S2).