Influenza virus neuraminidase (NA) is a homotetrameric surface protein that, in contrast to other non-influenza NAs, requires a quaternary assembly to exhibit enzymatic activity. Martiniano Bello presents MD simulations coupled to the MMGBSA method analysing the impact of tetramerization on the ligand recognition of avian N1 type NA. The monomeric and tetrameric, and closed and open-loop states, with and without the inhibitor oseltamivir and its natural substrate, sialic acid, are considered. The simulations indicate that the tetrameric state exerts dissimilar effects in binding affinity, characteristic of positive and negative cooperativity for oseltamivir and sialic acid, respectively.

(DOI: 10.1002/bip.23251)
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