

Description of Additional Supplementary Files

Supplementary Data 1. Parameters and scripts used in the MD simulation and in the analysis tools. Analyses were performed using python ≥ 3.7 , mdatanalysis $\geq 1.0.0$,seaborn $\geq 0.11.0$, scikit-learn $\geq 0.23.2$, scipy $\geq 1.5.2$. MD simulation parameters refer to those used in GROMACS 2019.4. Details are provided in the Methods section of the manuscript.