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MDPI

Supplementary information

Analysis of Different Binding Modes for Tiagabine within the GAT-1 Transporter

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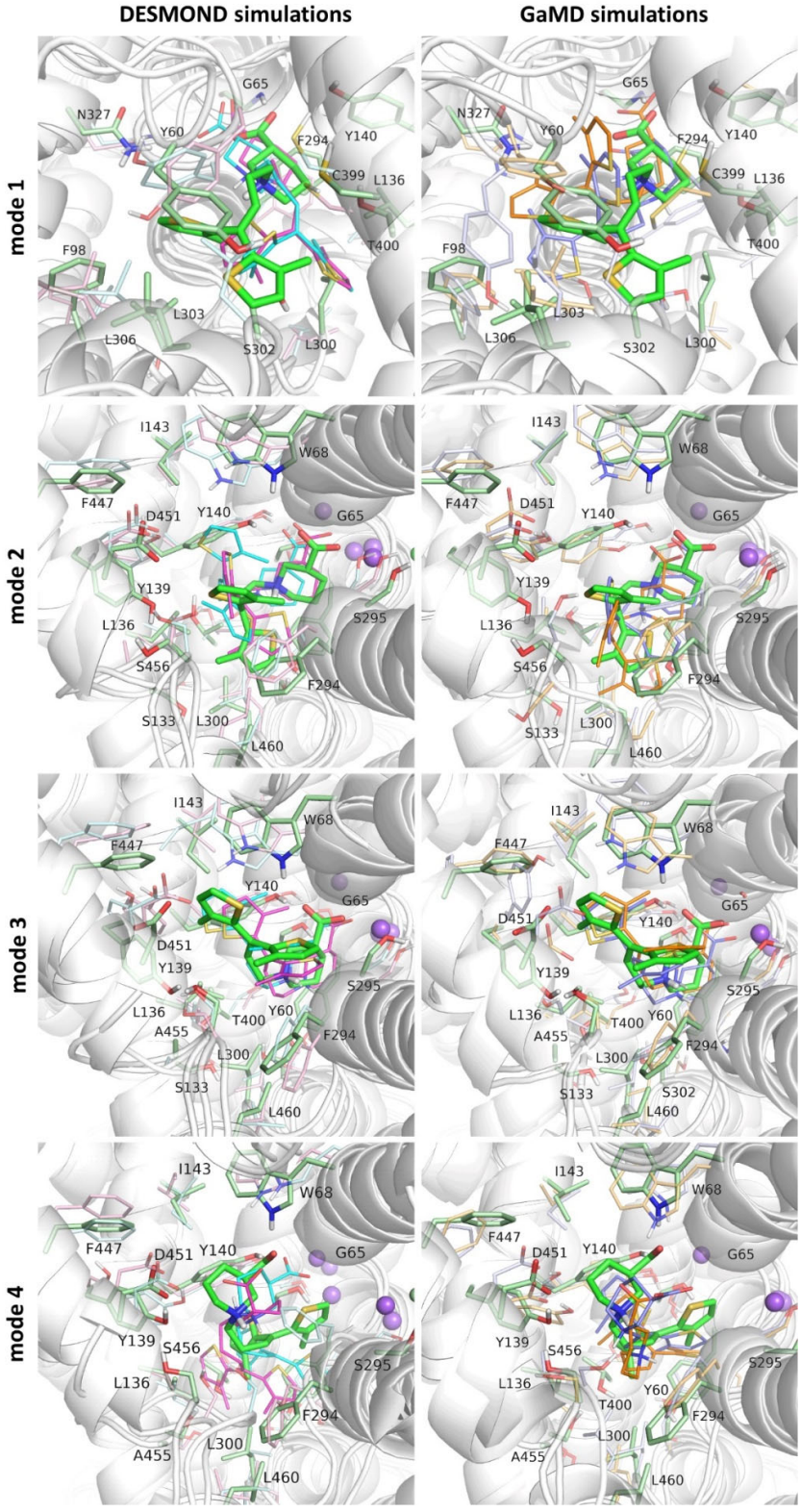

Figure S1. Investigated binding modes of tiagabine within hGAT-1, before (green) and after MD simulations (light blue – DESMOND MD 1; pink – DESMOND MD 2; light purple – GaMD 1; orange – GaMD 2).

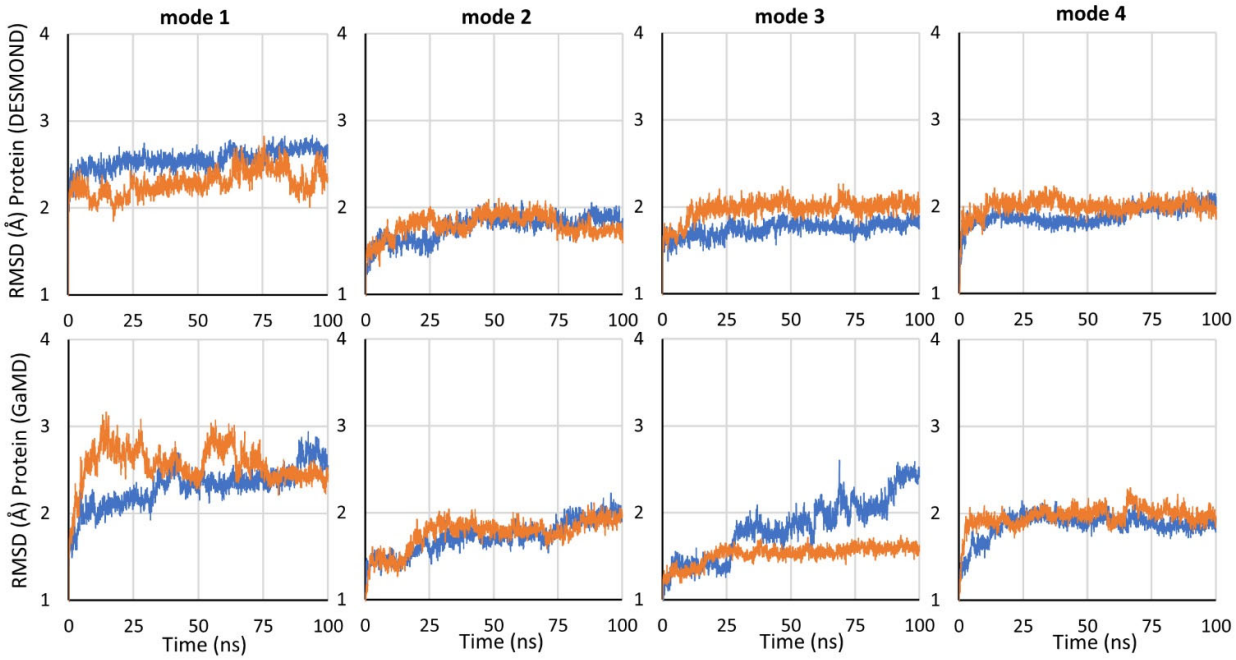

Figure S2. RMSD changes for hGAT-1 residues within 7 Å of tiagabine in different binding modes during molecular dynamics simulations carried out with DESMOND (classical MD) and NAMD (GaMD) programs.