

Figure S1. History of τ_1 , τ_2 , τ_3 , and τ_4 in **1** over the MD simulations starting from the docking pose.

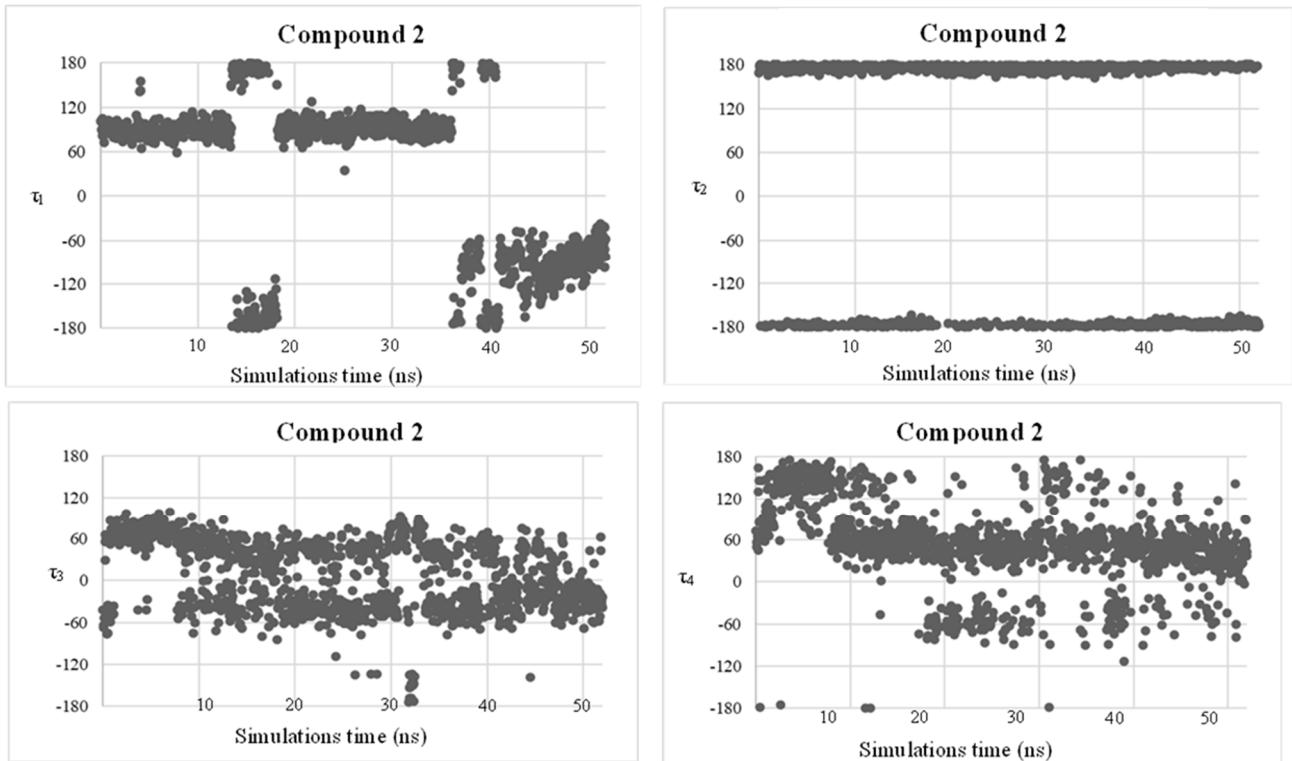


Figure S2. History of τ_1 , τ_2 , τ_3 , and τ_4 in **2** in the MD simulation starting from the docking pose.

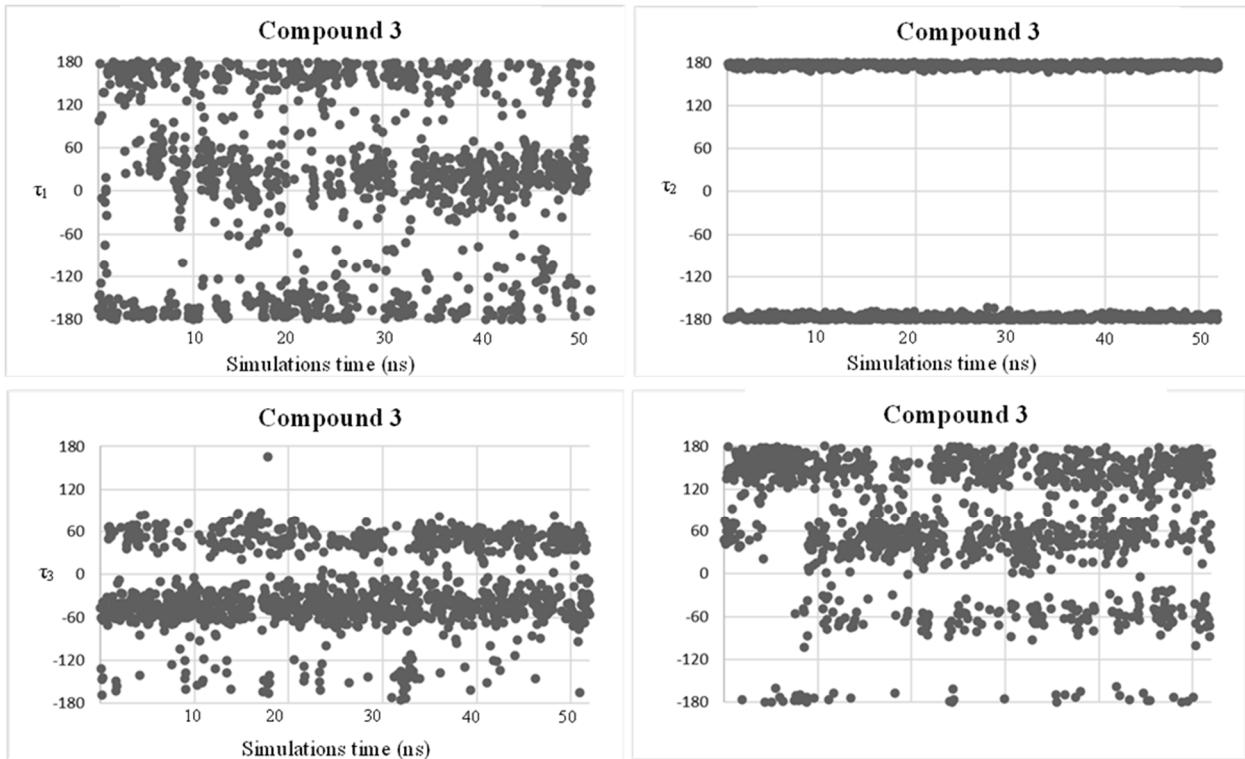


Figure S3. History of τ_1 , τ_2 , τ_3 , and τ_4 in **3** over the MD simulations starting from the docking pose.

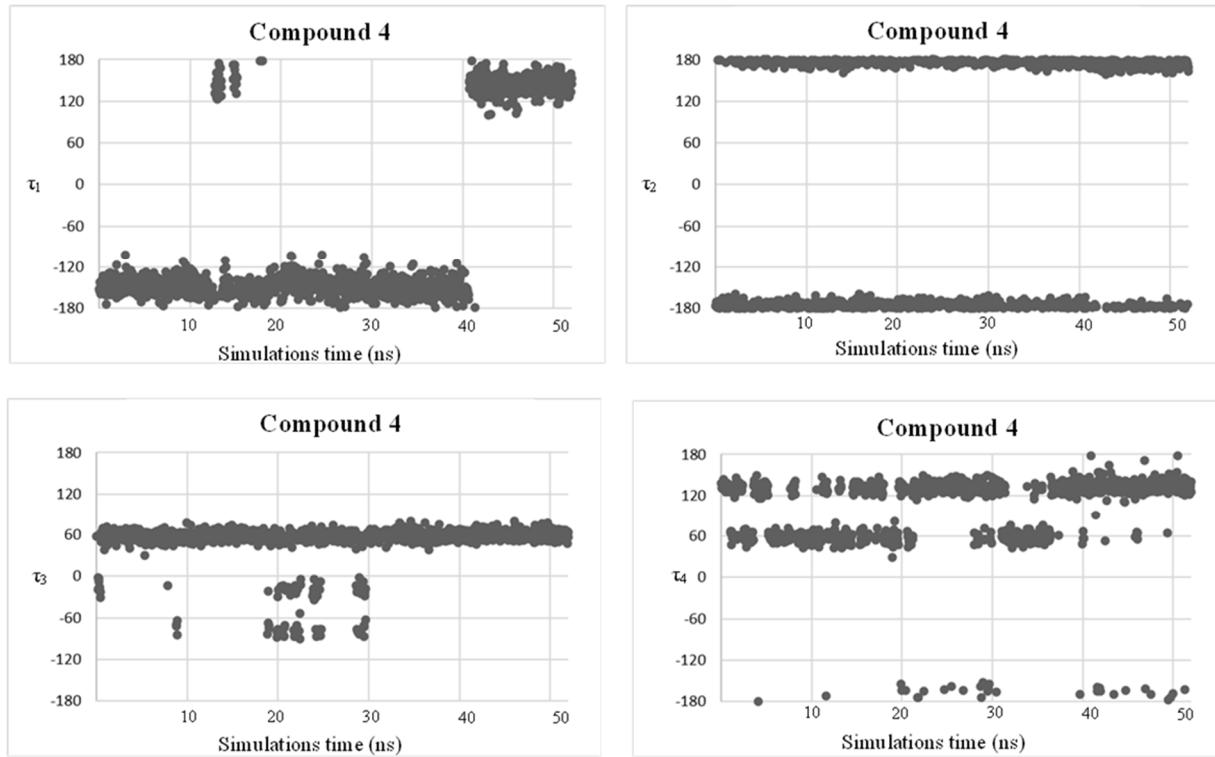


Figure S4. History of τ_1 , τ_2 , τ_3 , and τ_4 in **4** over the MD simulations starting from the docking pose.