

Abstract: The present work deals with the application of steered molecular dynamics simulations on medically interesting biomolecular systems. At first, methods for determining the free energy profile were tested on the $(Ala)_{10}$ model system. Then we focused on determining the free energy profile for binding of a ligand to the adenosine A_{2A} GPC receptor. We further studied the free energy profile associated with ion passage through the Gramicidin A ion channel. Finally, we applied this methodology to the TRPM2 ion channel.