At first, numerical integration algorithms was studied. Main objective was a study of active sites of HCV and HIV polymerases in complexes with a natural substrate and in complexes where an approaching nucleosidetriphosphate was replaced with inhibitors (S)-HMPMGpp and (S)-HMPMApp respectively. Further, an ABF method was used to obtain free energy profiles of water and methane molecules passing through a boundary between water and vacuum. Finally, the same method was used to obtain free energy profiles of water, methane and guanosine molecules passing through a lipid bilayer.