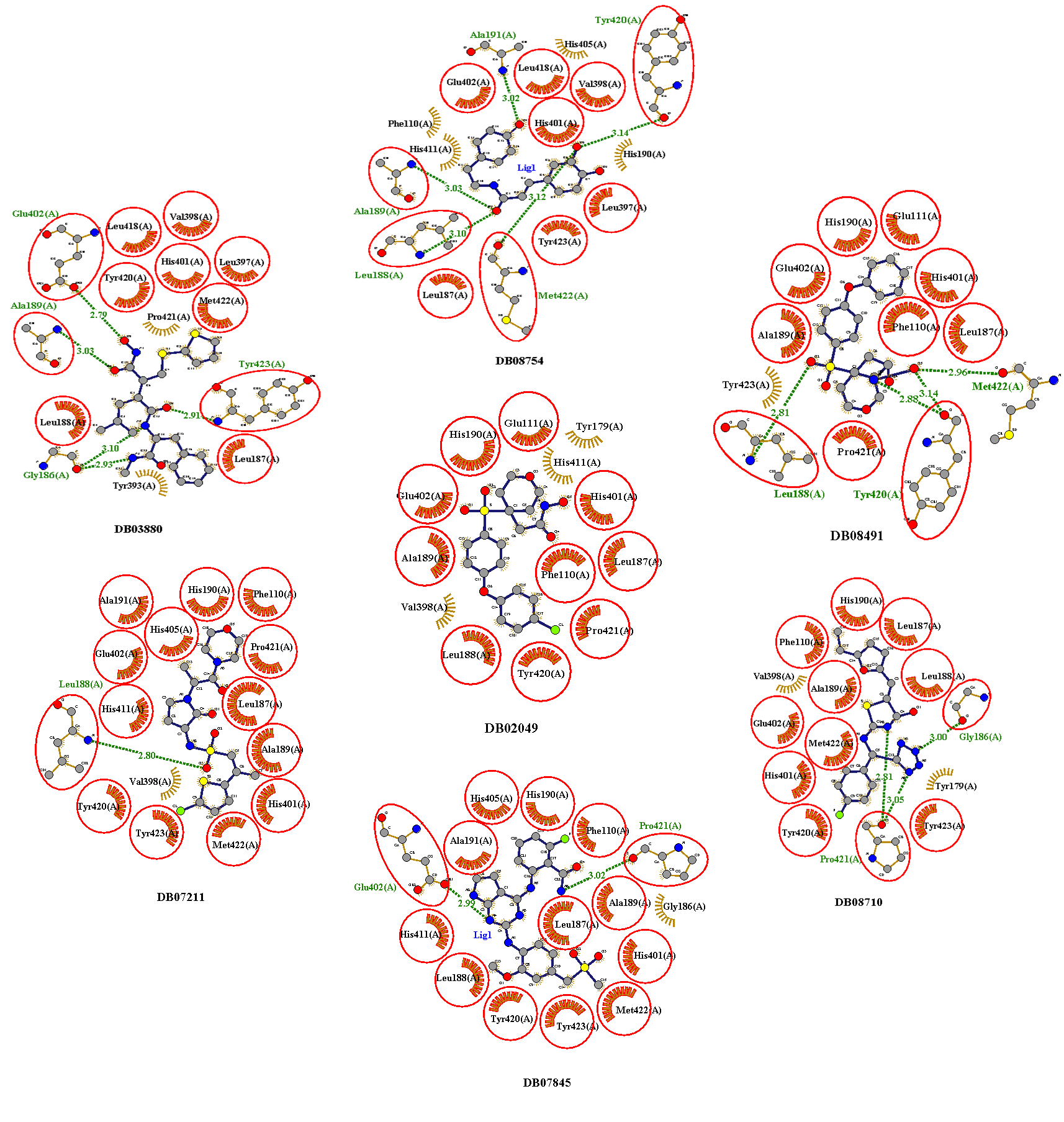
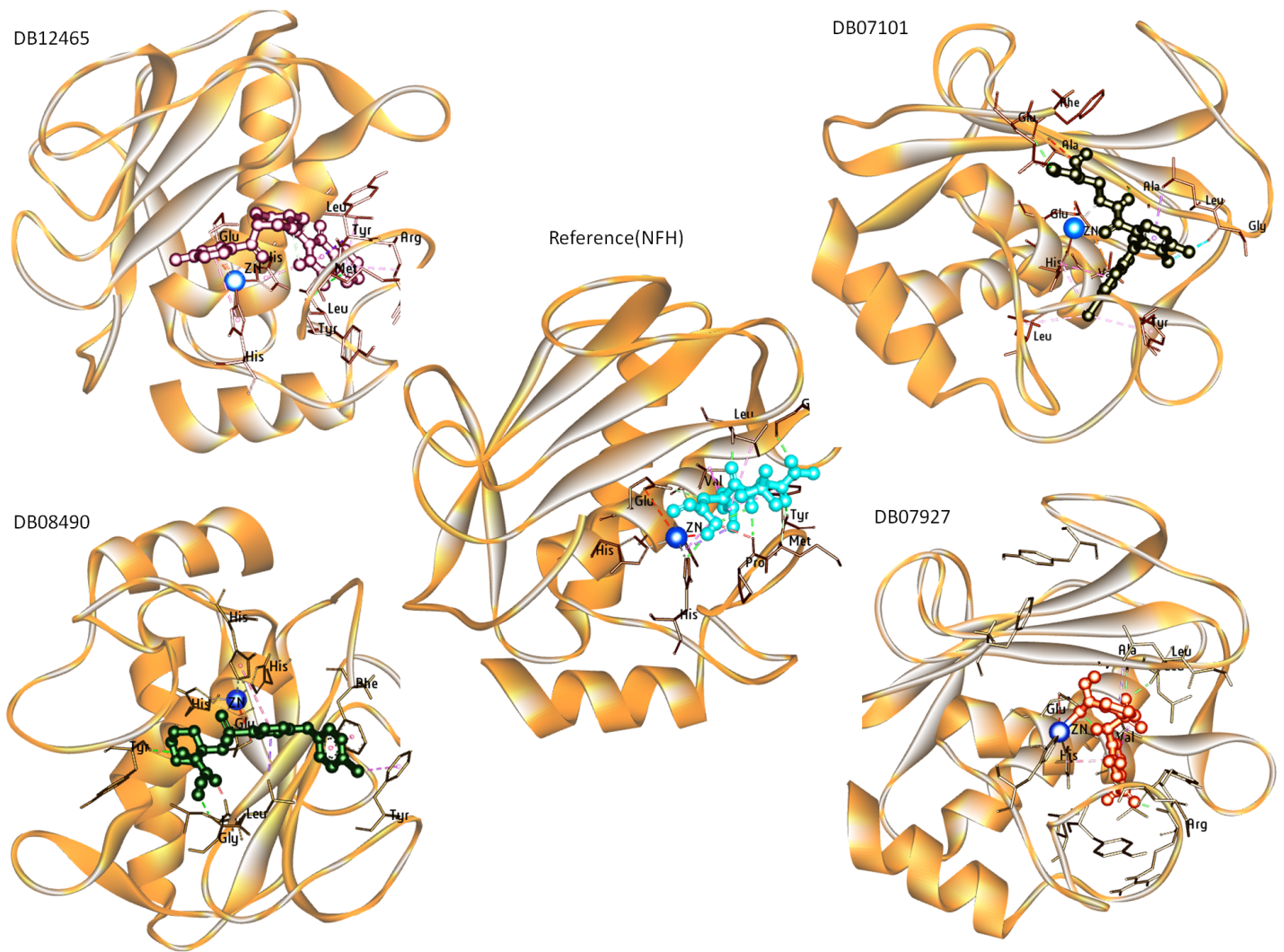


**Supplementary figure 1-** Total hit compounds screened by deeplearning method



**Supplementary figure 2-** 2D plots of top docked compounds not showing interaction with zinc



**Supplementary figure 3-** 3D plots of best four compounds and reference molecule after the 100 ns MD simulation