1. Loop RMSD vs overall MM-GBSA energy (for receptor only) through MM-GBSA analysis on MD trajectories.

I ran MM-GBSA calculations for MD trajectories of SIRT3/Inermediate/NAM complex that prepared from ternary complex 4FVT. The binding loop is changing from its original position. However, the energy fluctuation of the overall protein is too high and there is no correlation can be identified from the overall MM-GBSA energy plotted vs time.

To investigate the energetics associated with loop conformation change. I plan to use Prime to calculate single point energy for minimized structures with different loop conformation when Schrodinger license is available. The preparation of the loop conformation will be prepared using different constraints.

However, if the interest is in the residue contribution to the binding of C-pocket ligand, I plan to carry out loop refinement with the NAM in the C pocket and compare the binding energy for various loop conformations and mutations.

