

Captions to Movies

Movie A: Trajectory movie of a 100 ns unbiased MD simulation of the Δ - $\lambda\lambda\lambda\lambda$ complex showing the relatively fast interconversion of the torsion N3-C20-C19-N6 with a higher tendency to sample positive angles, and the more restricted conformational dynamics associated with the torsion N1-C15-C14-N4 in the 12-N-4 ring, which is in the negative range throughout the simulation. Non-polar hydrogen atoms are omitted for clarity.

Movie B: Trajectory movie of a 500 ns funnel metadynamics simulation to model the binding of [EuL²] to HSA. The protein is displayed as a transparent cartoon, Glu-184 and Glu-188 are shown as light-purple sticks, residues within 5 Å of [EuL²] are shown as light-purple thin wires, hydrogen bonds are blue dashed lines, and [EuL²] is shown as a ball-and-stick model, colored in cyan.

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And here is the link to this file for movie B

https://zenodo.org/records/15099016?token=eyJhbGciOiJIUzUxMiJ9.eyJpZCI6ImE1ZjE0N2ZkLWlyNjEtNDMwNS1iOTYyLWI0OWQ4MGJlY2YyNiIsImRhdGEiOnt9LCJyYW5kb20iOiIxN2MwZDliN2I3ODhkYmQ3MwYxODU0Y2FkNDk2ZW4yYyJ9.3TvgIx4VDL_q47NzicQghssTpXD_VT9CZTICgiovIBcn1JN-w7r5HfuOVauS1vN0PJedGrSTjNVOnR5W2aVLYA

Movie C: 360-degree spinning of the final model of the [EuL²]-HSA complex. The protein is displayed as a transparent cartoon, Glu-184 and Glu-188 are shown as light-purple sticks, residues within 5 Å of [EuL²] are shown as a light-purple thin wire, hydrogen bonds as blue dashed lines, and [EuL²] is shown as a ball-and-stick model colored in cyan. Non-polar hydrogens are hidden for clarity.