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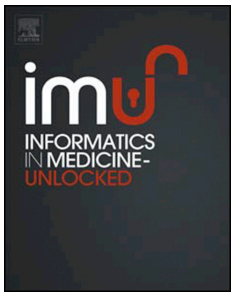

Investigations of binding mode insight in bacterial type-III secretion system tip protein (SipD): A molecular docking and molecular dynamics simulation study

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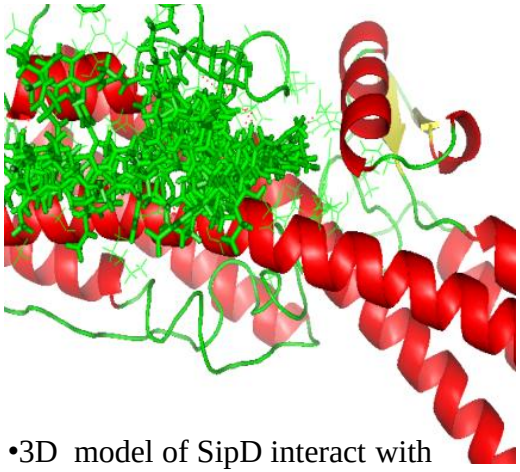
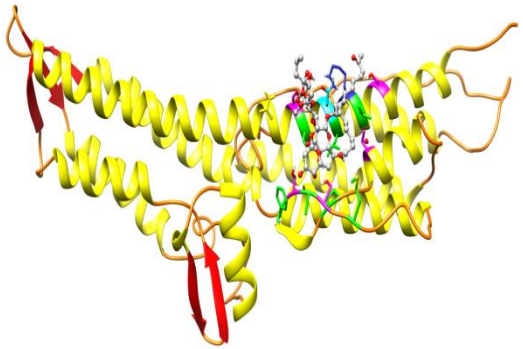
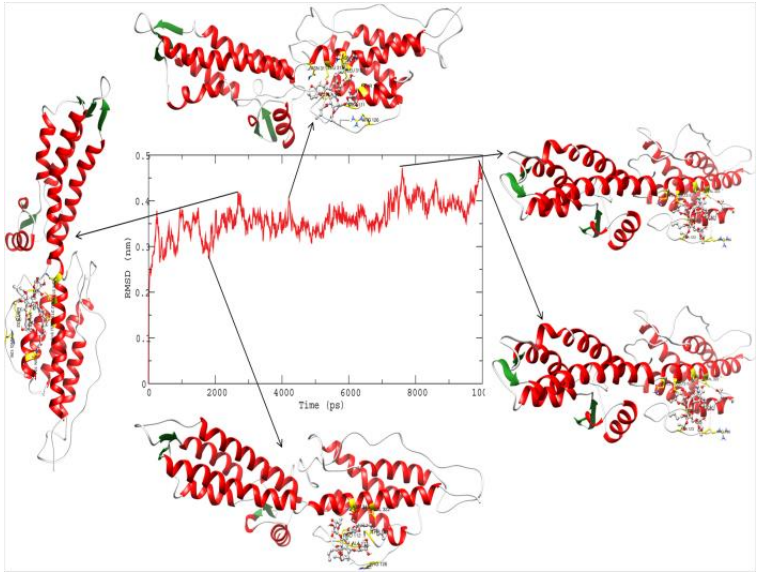


•3D model of SipD interact with TTSS inhibitors



• SipD interact with Caminoside A
• Higher G-score and reliable interaction



•The different conformational variations of SipD with Caminoside A by Molecular Dynamics Simulation