De novo design of selective Sortase-A Inhibitors: Synthesis, structural and in vitro characterization

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Abstract

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Novel molecules were designed against *Staphylococcus aureus* sortase A, an imperative and vital target involved in the bacterial virulence. Structure guided *de novo* designing was performed using different chemical fragments. These fragments were extended based on the requirements of the binding cavity. All the compounds in its binding orientation has formed good interaction network with amino acids HIS 120 and ARG 197. Molecules designed contain indole-chroman and indolin-chroman moieties and their docking scores were ranging from -6.92 to -5.67. Designed molecules were selected for synthesis and tested *in vitro* against *Staphylococcus aureus* sortase A using Fluorescence resonance energy transfer assay. The highest active molecule **KK4** ((*Z*)-3-((5-nitro-1*H*-indol-3-yl) methylene) chroman-2,4-dione)