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Development of antibacterial conjugates using sulfamethoxazole with monocyclic terpenes: a systematic medicinal chemistry based computational approach

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Highlights

- Development of novel antibacterial conjugate agents are described computationally combining sulfamethoxazole with 6 monoterpenes followed by azo-dye synthesis.
- Antibacterial activity of monoterpenes and proposed conjugates were evaluated computationally using molecular docking against target enzymes, DHPSs of 5 bacteria.
- Standardized drug-like parameters such as, Lipinski rule of five, toxicity and lethal dose values too are predicted computationally.
- This computational work helped to locate conjugates of sulfamethoxazole with thymol, and its synthesis and characterization as a new drug and *in vitro* tested against pathogenic bacteria with *in vivo* toxicity study.

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