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Comparative Modeling and Docking Studies for Identification of New Inhibitors against *Coxiella brunetii*

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ABSTRACT: Q fever is caused by the gram negative bacteria *Coxiella burnetii* which causes acute or chronic illness in human beings. This organism is an obligate parasite and belongs to coxiellaceae family. In recent years, Coxiella burnetii has acquired several mutations which have developed drug resistance against many effective antibiotics such as fluroquinolones. It drug is regarded as an important therapy against Q fever. Till date, the main mechanism of drug resistance is mutation in the quinolones resistance determining region (QRDR) which has appeared due to mutation in DNA gyrase protein sequence. To overcome this problem, new inhibitors are being identified which are effective against drug resistant bacteria. In this study, 3-dimensional structure of mutant protein has been modeled and new inhibitors against modeled structure have been determined. The amino acid sequence of DNA gyrase was retrieved from UniprotKb (Q83FD5). The protein sequence of DNA gyrase was modeled using MODELLER and further validated by several computational programs such as Ramachandaran plot, WHATIF and ProSA. Further, several databases were screened for lead identification and potential inhibitors were docked using Molegro. These computational methods are required for screening through large databases to identify inhibitor. This study will help in identification of potential inhibitors and drug discovery.

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