Cholera is a neglected disease with incidence worldwide. There are an increasing number of reports of *Vibrio cholerae* strains resistant to the current antibiotics, which demonstrate the urgency for new therapeutic alternatives. In this context, the enzyme alanine racemase is a well known protein present in this bacterium but absent in humans, making it an interesting target for the development of new drugs. The aim of this work was to modeling the structure of the enzyme alanine racemase from *V. cholerae* (*Vcholerae*AR) to use it as a drug target in virtual screening simulations (VS). The sequence of *Vcholerae*AR was obtained at UniProt database and modeled as a homodimer bonded to cofactor pyridoxal 5'-phosphate (PLP) and inhibitor D-cycloserine (4AX), through Modeller software. There were generated 1000 models and the best one was fully minimized by NAMD2 software for subsequent use in molecular dynamics simulations (MD) and VS. The library of natural products from Zinc database was used in VS through AutoDock and Molegro programs. The results of the 50ns MD for the protein in the Apo form or in the complex PLP-4AX, suggest that the presence of the ligands is needed to stabilize the quaternary fold and, the residues Arg128, Tyr341 and Met301 are the most important in the anchoring the inhibitor. The radius of gyration of protein-PLP-4AX complex remained stable throughout the simulation indicating that the presence of the ligands did not lead the protein to unfold. The virtual screening of 112,572 compounds with AutoDock program selected 317 of which six were found commonly by Molegro program. These six compounds were successfully filtered by ADMETox criteria and will be purchased for future *in vitro* tests. These results led to the identification of six drug hits with potential use against one of the most dispersed neglected diseases worldwide.

**Key words:** Alanine racemase; *Vibrio cholerae*; Molecular docking.

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