

## Abstract

The rise of multi-drug resistant bacterial strains has presented a challenge in the field of drug discovery and healthcare, with the discontinuation of now-ineffective treatments and the need to develop novel strategies in controlling diseases caused by pathogenic bacteria exemplified by *Escherichia coli* and *Salmonella enterica*. This report focused on delving into the possibility of compounds produced by the bacterial genus *Streptomyces* in inhibiting the shikimate pathway enzyme type I 3-dehydroquinase. The work involved a virtual screening and docking campaign against a collection of *Streptomyces*-produced compounds for their ability to inhibit type I 3-dehydroquinase. Although a bioactivity screening campaign, taking into consideration reported mechanisms of action of the screened compounds, revealed fumaramidmycin and xanthocidin as plausible candidates against the target enzyme, none were shown to be able to inhibit said enzyme owing to binding affinities and therefore inhibition constants lower than that of the natural ligand, 3-dehydroquinate. Nevertheless, it was revealed that negative binding affinities were obtained from the docking of xanthocidin with a model of type I 3-dehydroquinase from *Clostridioides difficile*, opening a possibility for modifications on the ligands to improve binding affinity towards said enzyme.