Structure-based prediction of Mycobacterium tuberculosis shikimate kinase inhibitors by high-throughput virtual screening.

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Abstract

A structure-based virtual screening protocol was used to predict Mycobacterium tuberculosis shikimate kinase (MtSk) inhibitors. Docking simulations were performed using eHiTS software and 644 drug-like compounds were identified as potential inhibitors. Forty-two percent of such inhibitors had a structural relationship to a triazole or a tetrazole heteroaromatic system which may provide a candidate lead for the discovery of MtSk inhibitors.