

DRUG DISCOVERY, DESIGNING CHEMISTRY AND PHARMACEUTICAL ANALYSIS &

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Tailored-pharmacophore model to enhance virtual screening and drug discovery: A case study on the identification of potential inhibitors against drug-resistant *Mycobacterium tuberculosis* (3R)-hydroxyacyl-ACP dehydratases

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Background: Virtual Screening (VS) is powerful tool in discovering molecular inhibitors which are most likely to bind to drug targets of interest. Herein, we introduce a novel VS approach, so-called “tailored-pharmacophore”, in order to explore inhibitors that overcome drug resistance.

Results/Methodology: The emergence and spread of drug resistance strains of tuberculosis is one of the most critical issues in health care. A tailored-pharmacophore approach was found promising to identify in silico predicted hit with better binding affinities in case of the resistance mutations in MtbHadAB as compared to thiacetazone, a prodrug used in the clinical treatment of TB.

Conclusions: This approach can potentially be enforced for the discovery and design of drugs against a wide range of resistance targets.

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