World Academy of Science, Engineering and Technology
International Journal of Medical and Health Sciences
Vol:12, No:05, 2018

Inhibition of 3-Deoxy-D-Arabino-Heptulosonate 7-Phosphate Synthase from Mycobacterium Tuberculosis Using High Throughput Virtual Screening and Molecular Dynamics Studies

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Abstract : Persistence of tuberculosis, emergence of multidrug-resistance and extensively drug-resistant forms of the disease, has increased the interest in developing new antitubercular drugs. Developing inhibitors for 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase from Mycobacterium tuberculosis (MtbDAH7Ps), an enzyme involved in shikimate pathway, gives a selective target for antitubercular agents. MtbDAH7Ps was screened against ZINC database, and shortlisted compounds were subjected to induce fit docking. Prime/Molecular Mechanics Generalized Born Surface Area calculation was used to validate the binding energy of ligand-protein complex. Molecular Dynamics analysis for of the lead compounds–MtbDAH7Ps complexes showed that the backbone of MtbDAH7Ps in their complexes were stable. These results suggest that the shortlisted lead compounds ZINC04097114, ZINC15163225, ZINC16857013, ZINC06275603, and ZINC05331260 could be developed into novel drug leads to inhibit DAH7Ps in Mycobacterium tuberculosis.

Keywords : MtbDAH7Ps, Mycobacterium tuberculosis, HTVS, molecular dynamics
Conference Title : ICT 2018 : International Conference on Tuberculosis
Conference Location : London, United Kingdom
Conference Dates : May 14-15, 2018