Title: Study of molecular interactions of the indole derivatives against RNA polymerase-binding protein (RbpA-Rv2050)

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Abstract:
Existing TB drugs are able to target actively growing bacteria through the inhibition of cell processes such as cell wall biosynthesis, DNA replication but fails to eliminate latent or dormant bacteria that survive inside the macrophages. In this study we targeted M.Tb. RNA polymerase- binding protein (RbpA-Rv2050) which is quite different than the usual targeting sites as it is responsible for mutations in TB bacteria and, also, alter the binding site. Here we applied QSAR, virtual screening, molecular modeling, molecular dynamics simulation and theoretical quantum

calculation approach for the discovery of effective indole ring containing lead moiety for its effective treatment. We applied 3-Dimentional QSAR and virtual screening techniques to curate the drug like candidates later we did molecular docking and molecular dynamic simulation study to make a short list of probably active compounds. Nextly, we calculate quantum descriptors by conducting TD-DFT calculation which give an idea about probability of the stability and reactivity of short listed compounds. We short listed a few promising indole derivatives which are potential to inhibit the RNAP function in M.Tb. bacteria.