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Molecular docking studies of some novel 2 & 3-(4-aminobenzamido) benzoic acid derivatives as DHFR inhibitors for treatment of tuberculosis

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Abstract : A Novel series 2 & 3-(4-aminobenzamido) benzoic acid derivatives were designed virtually considering the basic pharmacophore N-(3,5-bis (trifluoromethyl) phenyl)-5-chloro-2-hydroxybenzamide.The energy minimized conformers of each molecule was generated and docked with *M. tuberculosis* DHFR enzyme with PDB id: 1DF7 using Autodock 4.2.5.1. Most of the molecules have shown significant binding interaction with the receptor. Among the test compounds, **DX-35, DY-24, DX-18, DX-31 & DY-23** have shown highest free energy of binding -9.51 to -8.92 kcal/mol and also the very good estimated inhibitory constant in a range of 0.11 to 0.29 Ki μM, which is comparable to that of the reference standard methotrexate and the standard Anti-Tb drug Ciprofloxacin.
Keywords : Docking, Methotrexate, Ciprofloxacin, Autodock, Benzamide & Benzoic acid.

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