# Synthesis, docking Studies and antimicrobial evaluation of substituted hybrids of indole and benzothiazole.

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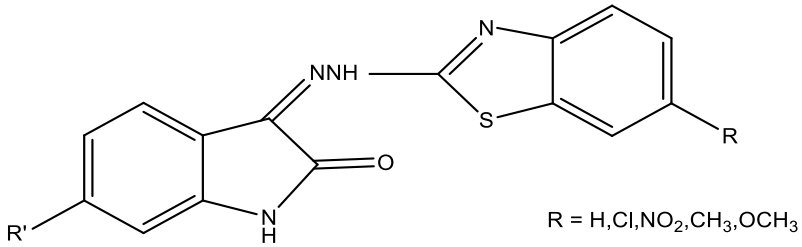
## Abstract:

A Series of 20 novel, substituted indole and benzothiazole hybrids incorporating 2-hydrazinyl benzothiazole derivatives were designed and synthesized using molecular hybridization. Molecular docking study was performed by using AUTODOCK 4.2 by taking the crystal structure of protein 3IVX (crystal structure of pantothenate synthetase in complex with 2-(2-(benzofuran-2-ylsulfonylcarbomoyl) -5-methoxy-1H-indol-1-yl)acetic acid) from Mycobacterium tuberculosis ( strain ATTCC 25618/H37Rϑ ). Some of the synthesized compounds exhibited promising activity **(MIC 1.13 – 64 µM)** against *Mycobacterium tuberculosis* H37Rϑ, MTB and MDR-TB first line drug resistant strain obtained from the patient using broth microdilution method, 1% Proportion method Middle brook 7H9 medium and with OADC supplement. Five of the evaluated compounds exhibited **MIC < 1.5µM**. Compound **(7) (R' = Me and R = $NO_2$)** and **(16) (R'=$NO_2$ and R=Me )** showed **MIC of 1.131µM** compared to the standards **isoniazid (0.28µM), Rifampicin(0.09µM), Streptomycin(2µM) and Ethambutol (4µM)**.The compound **(16) (R'=$NO_2$ and R= Me)** exhibited highest binding energy of **-7.26 K cal/mol** having interaction with Glu 189, Ser 196 and Arg 207 of target pantothenate synthetase. *In vitro* studies and docking studies for antibacterial and anti-fungal agents against four bacteria (Staphylococcus aureus, Bacillus substillis, Escherichia coli and Klebsheilla peneumoneae and three fungi (Aspergillug niger, Candida albicans and Saccharomycescereveseae) using the standards **Streptomycin, Ciprofloxacin and Ketoconozole** respectively was done. Majority of the compounds were found to possess a significant broad spectrum antibacterial activity **(10.0-40.0 mm)** of zoneof Inhibition against four bacteria (Staphylococcus aureus, Bacillus substillis, Escherichia coli and Klebsheilla peneumoneae) by comparing with **Streptomycin (25-45.5mm) and Ciprofloxacin (40.0-46.9 mm).** In **a**ntifungal activity some of the compounds showed the zone of inhibition **(10.0-45.0 mm)** against three fungi (Aspergillug niger, Candida albicans and Saccharomycescereveseae) by taking the standard **Ketoconozole** which showed the zone of inhibition( **35.0-55.5mm).**




**General structure-I**

**Keywords:**

**Anti-tubercular, antibacterial, antifungal,Benzothiazole, Indole.**