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Computer-aided drug design and analysis of some isonicotinic hydrazide-derived analogues against Mycobacterium Tuberculosis targets (3igo.pdb and 4duh.pdb)

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Abstract

Isonicotinic acid hydrazide (INH) is the most important drug in the therapy of tuberculosis but not without some serious side effects. Therefore, with the use of computer aided drug design, the free amino group (-NH_2) present in INH was condensed with various carbonyl compounds to form hydrazones-Schiff bases. These hydrazones were further converted into thiazolidinones by the addition of thiaglycolic acid. As shown in Fig. 1 and 2, molecular docking studies of the designed compounds reveal that all the analogues possess better binding affinity (INH-140: -6.4Kcal/mol, INH-360: -6.5Kcal/mol,) compared to parent compound-INH (INH-78: -5.1Kcal/mol) at the target proteins (3igo.pdb and 4duh.pdb). INH exhibited a better PA (prediction activity) score compared to the designed analogues but all the analogues show less toxicity potential relatively.

Biography:

Naruka. S. Y is a Pharmacist (BPharm) with a Masters' degree in Pharmaceutical and Medicinal Chemistry. Presently, he is a lecturer and researcher in the Department of Pharmaceutical and Medicinal Chemistry, University of Jos Nigeria. He is highly interested and passionate about Medicinal Chemistry with special focus in Drug Development, Design and Synthesis. He has published over seven (7) papers in reputable journals

Speaker Publications:

1. "Design, Molecular Docking And In Silico Analysis Of Analogues Of Chloroquine And Hydroxychloroquine Against SARs-COV-2 Target (6w63.pdb)"
2. "Synthesis and antimicrobial their corresponding 1,3"
3. "Pharmacognostic, acute toxicity, and analgesic studies of the stem of Guiera Senegalensis j.f gmel (combretaceae)"
4. "Antimicrobial activity and characterization of seven synthetic formamidine disulfide derivatives"
5. "Synthesis and characterization of Formamidine disulfide schiff bases and their corresponding 1"

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