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Re-Purposing of FDA approve drugs for tuberculosis treatment

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Tuberculosis is one of the most prevalent infections of human beings and it contributes considerably to illness and even death around the Global . It spread by inhaling tiny droplets of saliva from the cough or sneezes of an infected person .

It affects long parenchyma which is caused by *Mycobacterium Tuberculosis* currently , India is the highest Tb burden country in the world , Home to 20% off cases occurring globally because of TB, maximum people are dying every year approximately 0.37 million in India itself.

Drug repurposing is approach of promise known drugs are examined for a new indication . The trial site has been attempted to identify drugs that could target MurB and MurE enzymes which involved in the muramic acid synthesis pathway in mycobacterium tuberculosis. FDA approve drugs from two repositories 1. Drug Bank 2. e-LEA3 were screened against these enzymes .
several point of references were applied to study the protein drug interactions.

The trial site found a sulfadoxine (-7.3 kcal/mol) and pyrimethmine (-7.8kcal /mol) to show stable interactions with MurB while sildenafil(-9.1kcal/mol) and lifitegrast (-10.5kcal/mol) showed most reliable interaction with MurE . Hence ,these drugs for repurposing has expanded and they have focused on the molecular docking based virtual screening of 10 FDA approved drugs . They used to treat bacterial infections against target methoxy mycolic acid synthesis 4(MMA4) and Cyclopropane mycolic acid synthesis (CmaA2) .

The 10 FDA approved drugs are cefpodoxime avibactum , lymecycline , clofazimine , meropenem clavulanate , 6-fluoroquinolone sulbactum cephalosporin and tazobactum for target MMA4 drugs . For target cmaA2 drugs , lymecycline , clofazimine and tazobactum with binding energy -15.46 -12.80 and-10.48 identified as a top potential drug with well binding interactions .

Molecular docking analysis dispose out that lymecycline interacts well with the target MMA4 and CmaA2 with a low binding energy of -9.66 and -15.46 . By the virtual screening significant they predict that lymecycline acts a strong inhibitor and interrupt the function of target gene MMA4 and CmaA2 .

Among the 10 FDA approved drugs to identify the best inhibitors against two target MMA4 and CmaA2 , which involves in oxygenated mycolic acid synthesis of mycobacterium tuberculosis by performing virtual ligand based screening results that lymecycline will be potential drug with lower binding energy value -9.66 and -15.46 against target MMA4 and CmaA2 respectively.

References

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