PENAMBATAN MOLEKUL SENYAWA BIOAKTIF FLAVONOID TERHADAP RNA-*POLYMERASE Mycobacterium tuberculosis*

Abstrak

Tuberkulosis masih merupakan salah satu penyakit yang mematikan di Dunia. Di tahun 2013, sekitar 9 juta jiwa terjangkit TB dan 1,5 juta meninggal akibat penyakit ini. Pada penelitian ini penulis membahas tentang interaksi antara senyawa bioaktif flavonoid dengan reseptor RNA *polymerase* secara In Silico. Pertama-tama, modeling homology untuk mendapatkan struktur senyawa tiga dimensi dari RNA polymerase *Mycobacterium tuberculosis* dan preparasi keenam senyawa aktif flavonoid yang akan menjadi ligan dengan rifapentin sebagai pembanding. Keenam senyawa bioaktif flavonoid dan rifapentin di docking kan dengan sub unit beta RNA *polymerase* hingga diperoleh energi ikatan. Keenam senyawa bioaktif flavonoid dan rifapentin di dockingkan menggunakan software yaitu PLANTS. Keenam senyawa bioaktif flavonoid dan rifapentin berikatan disisi aktif subunit β RNA *polymerase*, mekanisme dari model untuk menginhibitor RNA *polymerase* yang mana keenam senyawa bioaktif flavonoid dan rifapentin memblok sintesa RNA secara *steric* sehingga RNA yang dihasilkan panjangnya terdiri dari tiga nukleotida ("steric-occlusion model")

Hasil : Luteolin dan rutin memiliki nilai energi ikatan lebih kecil dari rifapentin, Luteolin dan rutin juga diprediksi memiliki afinitas ikatan yang sangat baik terhadap RNA *polymerase Mycobacterium tuberculosis*

Kata kunci : Tuberkulosis, RNA polymerase, Flavonoids, Antituberkulosis, Docking

MOLECULAR DOCKING STUDIES OF FLAVONOID BIOACTIVE COMPOUND AGAINST RNA POLYMERASE *MYCOBACTERIUM TUBERCULOSIS*

Abstract

Tuberculosis (TB) remains one of the world's deadliest communicable diseases. In 2013, an estimated 9 million people developed TB and 1.5 million died from the disease. In this research we studied the bioactive compounds of flavonoid-RNA Polymerase receptor interactions In silico. First, homology modeling was performed to obtain the three dimensional structure of RNA Polymerase *Mycobacterium tuberculosis* and preparation of sixth bioactive compounds of flavonoid which will be as ligands with rifapentine as a comparison. The sixth bioactive compounds of flavonoid and rifapentine were docked with beta subunit of RNA polymerase *Mycobacterium tuberculosis* until energy binding values were obtained. The sixth bioactive compounds of flavonoid, and rifapentine were docked with software PLANTS. The sixth bioactive compounds of flavonoid, and rifapentine binds to active site on the β-subunit RNA polymerase, the mechanism model for inhibition of RNA polymerase in which sixth bioactive compounds of flavonoid and rifapentine sterically block synthesis of an RNA product longer than three nucleotides ("steric-occlusion model")

Result : Luteolin and Rutin had lesser energy binding values than rifapentine and luteolin and rutin also predicted to have greater binding affinity to RNA polymerase *Mycobacterium tuberculosis*

Keywords: Tuberculosis, RNA polymerase, Flavonoids, Antituberculosis, Docking


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