

INTISARI

ARWianto, D., 2013, STUDI INTERAKSI IN SILICO senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin TERHADAP ENZIM DIHIDROFOLAT REDUKTASE PADA BAKTERI DAN SEL MAMALIA, SKRIPSI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA.

Senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin dilaporkan mempunyai aktivitas penghambat enzim dihidrofolat reduktase pada bakteri dan sel mamalia sehingga memberikan efek antimetabolit. STUDI INTERAKSI IN SILICO senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin terhadap enzim DHFR diperlukan untuk mengetahui afinitas dan pola interaksi antara senyawa diatas dengan DHFR bakteri dan DHFR sel mamalia. Penelitian ini bertujuan untuk mengetahui afinitas dan pola interaksi senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin terhadap bakteri dan sel mamalia.

Senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin dioptimasi geometri menggunakan perangkat lunak Hyperchem selanjutnya dilakukan dengan cara preparasi target, preparasi ligan, validasi metode *docking*, dan analisis *docking* menggunakan *autodock vina* sehingga didapatkan interaksi ligan dengan target, energi bebas pengikatan, ikatan hidrogen, dan pola interaksi.

Afinitas dari senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin lebih tinggi bakteri dibandingkan sel mamalia. Pola interaksi dilihat pada lima belas senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin dengan enzim DHFR bakteri menunjukkan ikatan hidrogen dengan asam amino Asp31A dan DHFR sel mamalia menunjukkan ikatan hidrogen dengan asam amino Glu30A dan Val115A.

Kata kunci : DHFR bakteri dan sel mamalia, Hyperchem, PyRx, Studi Interaksi

ABSTRACT

ARWianto, D., 2013, INTERACTION STUDY DERIVED COMPOUNDS ON 2,4-DIAMINOPIRIDO [2,3-d] PYRIMIDINE WITH DIHIDROFOLAT ENZYME IN BACTERIA AND MAMMALIAN CELLS, THESIS, FACULTY OF PHARMACY, UNIVERSITY OF SETIA BUDI, SURAKARTA.

DERIVED COMPOUNDS 2,4-DIAMINOPIRIDO [2,3-d] pyrimidine was reported to have dihidrofolat reductase enzyme inhibitory activity in bacteria and mammalian cells that give effect antimetabolite. STUDY THEIR INTERACTION IN COMPOUND 2,4-silico DIAMINOPIRIDO [2,3-d] pyrimidine against DHFR enzymes necessary to determine the affinity and interaction patterns between the above compounds with bacterial DHFR and DHFR mammalian cells. This study aims to determine the affinity and interaction patterns DERIVED COMPOUNDS 2,4-DIAMINOPIRIDO [2,3-d] pyrimidine against bacteria and mammalian cells.

DERIVED COMPOUNDS 2,4-DIAMINOPIRIDO [2,3-d] pyrimidine geometry optimized using Hyperchem software then performed by way of target preparation, ligand preparation, docking method validation, and analysis of docking using AutoDock vina so we get to the target ligand interactions, free energy bonding, hydrogen bonding, and interaction patterns.

Affinity of 2,4-DERIVED COMPOUNDS DIAMINOPIRIDO [2,3-d] pyrimidine higher bacteria than mammalian cells. Interaction pattern seen in sixteen 2,4-DERIVED COMPOUNDS DIAMINOPIRIDO [2,3-d] pyrimidine with bacterial DHFR enzyme showed hydrogen bonding with amino acids and DHFR Asp31A mammalian cells indicate hydrogen bonds with amino acids and Val115A Glu30A.

Keywords: DHFR bacteria and mammalian cells, Hyperchem, PyRx, Interaction Studies