ABSTRAK

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Judul : *Molecular Docking* Senyawa Caboxamycin Pada *Mycobacterium tuberculosis Polyketide Synthase 13* (Pks13)

Senyawa caboxamycin merupakan antibiotik baru yang termasuk dalam kelompok *benzoxazole* yang diproduksi dari *Streptomyces* sp. NTK 937 (*marine strain*). Penelitian ini bertujuan untuk mengetahui mekanisme penghambatan senyawa caboxamycin terhadap *Mycobacterium tuberculosis polyketide synthase 13* (Pks13) secara *in silico* dengan metode *molecular docking*. Tahapan *Molecular docking* dimulai dengan optimasi struktur senyawa caboxamycin 3D, preparasi protein *polyketide synthase 13* (Pks13), validasi metode, dan *docking* senyawa caboxamycin yang teroptimasi pada protein *Mycobacterium tuberculosis polyketide synthase 13* (Pks13). Hasil *docking* protein *Mycobacterium tuberculosis polyketide synthase 13* (Pks13) pada ligan standard adalah -144,0 kkal/mol, pada streptomisin adalah -101,7 kkal/mol, dan pada caboxamycin adalah -75,9 kkal/mol. Streptomisin dan caboxamycin memiliki ikatan hidrogen yang sama terhadap residu asam amino protein *Mycobacterium tuberculosis polyketide synthase 13* (Pks13) yaitu ASN-1640 dan HIS-1664, sehingga caboxamycin memiliki mekanisme kerja dalam menghambat *polyketide synthase 13* (Pks13) pada *Mycobacterium tuberculosis* secara *in silico*. Senyawa caboxamycin memiliki mekanisme molekuler dalam menghambat protein *Mycobacterium tuberculosis polyketide synthase 13* (Pks13) yang ditunjukkan dengan adanya pembentukkan ikatan hidrogen. Sehingga senyawa caboxamycin berpotensi sebagai antituberkulosis secara *in silico*.

Kata kunci :

Molecular docking, *in silico*, Pks13, caboxamycin, tuberkulosis

ABSTRACT

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Title : Molecular Docking Of Caboxamycin On Mycobacterium tuberculosis Polyketide Synthase 13 (Pks13)

Caboxamycin is a new antibiotic benzoxazole group produced from *Streptomyces* sp. NTK 937 (marine strain). This study aims to determine the mechanism of inhibition of Caboxamycin compounds against *Mycobacterium tuberculosis* polyketide synthase 13 (Pks13) in silico with molecular docking method. Molecular docking stage begins with optimization of structure of caboxamycin 3D compound, preparation of the protein polyketide synthase 13 (Pks13), method validation, and docking of optimized caboxamycin compound on the Mycobacterium tuberculosis polyketide synthase 13 (Pks13) protein. Docking result for Mycobacterium tuberculosis polyketide synthase 13 (Pks13) protein on standard ligand was -144.0 kcal/mol, streptomycin was -101.7 kcal/mol, and caboxamycin was -75.9 kcal/mol. Streptomycin and caboxamycin have the same hydrogen bonds to amino acid residues of Mycobacterium tuberculosis polyketide synthase 13 (Pks13) protein, namely ASN-1640 and HIS-1664, that caboxamycin has a mechanism of action in inhibiting polyketide synthase 13 (Pks13) in Mycobacterium tuberculosis in silico. caboxamycin compound has a molecular mechanism in inhibiting *Mycobacterium tuberculosis* polyketide synthase 13 (Pks13) protein which is indicated by the formation of hydrogen bonds. Caboxamycin compound has the potential as an antituberculosis in silico.

Keywords:

Molecular docking, in silico, Pks13, caboxamycin, tuberculosis