ABSTRAK

Serial turunan dari senyawa 3,4-dimetoksi-β-nitrostirena telah berhasil disintesis melalui reaksi kondensasi nitroaldol (reaksi Henry), termasuk senyawa baru 3,4-etilendioksi-β-bromo-β-nitrostirena (**6**) dengan rendemen dan komposisi isomer *E* dan *Z* yang bervariasi. Uji pendahuluan antimikroba terhadap *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Candida albicans*, dan *Aspergillus niger* telah dilakukan pada senyawa hasil sintesis yang terpilih berdasar studi literatur dan kajian *docking* molekuler dengan reseptor *protein phosphatase*. Uji antimikroba dilakukan menggunakan metode dilusi pada bakteri dan yeast serta metode difusi pada kapang. Uji aktivitas antioksidan menggunakan ABTS dan uji penghambatan enzim α-glukosidase juga telah dilakukan. Dalam rangka mengetahui efek modifikasi rantai alkildioksi pada posisi 3,4 cincin benzena dan perubahan substituen pada karbon-β terhadap bioaktivitas senyawa turunan ini, maka telah dilakukan uji aktivitas antimikroba pada mikroba terpilih beradasarkan nilai MIC terendah serta uji *in silico* terhadap protein tyrosine phosphatase 1B (PTP1B) baik secara *docking* molekuler maupun simulasi dinamika molekuler. Pada bakteri, Senyawa 3,4-dimetoksi-β-metil-β-nitrostirena (**2**) memiliki kemampuan menghambat pertumbuhan bakteri Gram positif lebih baik dibandingkan terhadap bakteri Gram negatif. Namun, secara umum aktivitas tertinggi ada pada *yeast*. Senyawa 3,4-dimetoksi-β-metil-β-nitrostirena (**2**) hasil sintesis memiliki aktivitas yang relatif rendah sebagai penghambat enzim α-glukosidase maupun sebagai antioksidan. Senyawa 3,4-etilendioksi-β-nitrostirena (**4**) dan 3,4-etilendioksi-β-metil-β-nitrostirena (**5**) memiliki aktivitas tertinggi terhadap *Candida albicans*. Kedua senyawa tersebut beserta senyawa 3,4-dimetoksi-β-metil-β-nitrostirena (**2**) juga berpotensi sebagai kandidat inhibitor PTP1B berdasarkan kajian *docking* molekuler. Namun, senyawa 3,4-etilendioksi-β-metil-β-nitrostirena (**5**) lebih direkomendasikan sebagai struktur paling potensial untuk agen antimikroba sekaligus menjadi bagian dari fragmen penghambat PTP1B.

ABSTRACT

A derivative series of 3,4-dimethoxy-β-nitrostyrene was synthesized through nitroaldol condensation (Henry reaction), including a new compound of 3,4-ethylenedioxy-β-bromo-β-nitrostyrene (**6**) with varying yields and conpositions of *E* and *Z* isomers.. A preliminary assays of antimicrobial activity against *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Candida albicans*, and *Aspergillus niger* were performed on synthesized compound selected according to literature and docking studies with *protein phosphatase* receptors. The antimicrobial assays were carried out using dilution method on bacteria and yeast and diffusion method on mold. Antioxidant activity assay using ABTS and α-glucosidase inhibiton assay were also undertaken. In order to determine the effect of modification of the alkyldioxy chain at the position 3,4 of the benzene ring and the change of the substituent at β-carbon on the bioactivity of the studied compounds, assays the antimicrobial activity against the selected strain based on the lowest MIC value and *in silico* studies on protein tyrosine phosphatase 1B (PTP1B) using molecular docking and molecular dynamic simulation were carried out. In bacteria, 3,4-dimethoxy-β-methyl-β-nitrostyrene (**2**) were more potent against Gram-positive bacteria than Gram-negative bacteria. Among the micriobial strains, its highest activity against yeast. The compound had relatively low activity as an inhibitor of α-glucosidase and as antioxidant. 3,4-Ethylenedioxy-β-nitrostyrene (**4**) and 3,4-ethylenedioxy-β-methyl-β-nitrostyrene (**5**) had the highest activity against *Candida albicans*. The two compounds along with 3,4-dimethoxy-β-methyl-β-nitrostyrene (**2**) were also potential as candidate PTP1B inhibitor according to molecular docking studies. However, 3,4-ethylenedioxy-β-methyl-β-nitrostyrene (**5**) was recommended as the most potential structure for antimicrobial agent as well as being part of the fragment of PTP1B inhibitor.