INTISARI

DESAIN SENYAWA TURUNAN 2-METILTIO-5-(4-AMINO-2-METILPIRIMIDIN-5-IL)-1,3,4-OXADIAZOL SEBAGAI ANTI-*TOBACCO MOSAIC VIRUS* (TMV) BERDASARKAN HASIL ANALISIS HUBUNGAN KUANTITATIF STRUKTUR-AKTIVITAS (HKSA)

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Desain senyawa turunan 2-metiltio-5-(4-amino-2-metilpirimidin-5-il)-1,3,4-oxadiazole sebagai anti-*tobacco mosaic virus* (TMV) dilakukan berdasarkan model hubungan kuantitatif struktur-aktivitas (HKSA) yang diperoleh dari hasil perhitungan deskriptor dengan metode semiempiris model PM6. Metode regresi multilinear (MLR) dan jaringan syaraf tiruan (JST) digunakan untuk menganalisis model HKSA dan memprediksi tingkat aktivitas EC_{50}.

Analisis HKSA dengan menggunakan metode MLR didapatkan persamaan terbaik yaitu log EC_{50} = -87,673 – 306,866 QC_5 + 138,610 E_{HOMO} + 0,222 HE + 0,796 log P – 0,022MW, dengan parameter statistik n = 15, r^2 = 0,680, SEE = 0,152, F_{hit}/F_{tab} = 1,054. Desain HKSA melalui analisis JST diperoleh arsitektur optimum 24-17-1. Desain dan nilai aktivitas senyawa yang diusulkan dari kedua metode analisis ini adalah 2-Bromobenziltio-5(4-amino-2-metilpirimidin-5-il)1,3,4-oxadiazol dengan EC_{50} = 58,65 µg/mL menggunakan model MLR dan EC_{50} = 15,17 µg/mL melalui model JST dan 2-Iodobenziltio-5(4-amino-2-metilpirimidin-5-il)1,3,4-oxadiazol dengan EC_{50}= 6,17 µg/mL menggunakan model MLR dan EC_{50} = 10,25 µg/mL melalui metode JST.

Kata kunci: 1,3,4-oxadiazol, anti TMV, HKSA, PM6

ABSTRACT

DESIGN OF 2-METHYLTHIO-5-(4-AMINO-2-METHYLPYRIMIDIN-5-YL)-1,3,4-OXADIAZOLE DERIVATIVES FOR ANTI TOBACCO MOSAIC VIRUS (TMV) BASED ON QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) ANALYSIS

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Design of 2-methylthio-5-(4- amino-2-methylpyrimidin-5-yl)-1,3,4-oxadiazole derivative compounds as an anti-TMV based on QSAR analysis obtained from the calculation of descriptor using semiempirical methode PM6 has been done. The MLR and ANN methods are used to obtain the QSAR model and predict its EC_{50} activity.

Analysis of QSAR by using MLR method give the best equation log EC_{50}= -87,673 – 306,866 QC_5 + 138,610 E_{HOMO} + 0,222 HE + 0,796 log P – 0,022MW, with statistical parameter n = 15, r^2 = 0,680, SEE = 0,152, F_{hit}/F_{tab} = 1,054. Meanwhile QSAR analysis using ANN methode provide the optimum architecture of 24-17-1. The new design and activity value of the proposed compounds by using the two methods are 2-Bromobenzilthio-5(4-amino-2-methylpirimidin-5-yl)1,3,4-oxadiazole with EC_{50} activity value of 58,65 µg/mL using the MLR method and EC_{50} of 15,17 µg/mL using the ANN methode and 2-Iodobenziltio-5(-4-amino-2-metilpirimidin-5-il)1,3,4-oxadiazole with activity value EC_{50} of 6,17 µg/mL using the MLR method and EC_{50} of 10,25 µg/mL using the ANN method.

Keywords: 1,3,4-Oxadiazole, anti-TMV, QSAR, PM6