DESAIN SENYAWA ANTIKANKER TURUNAN BENZOILHIDRAZON BERDASARKAN ANALISIS HUBUNGAN KUANTITATIF STRUKTUR AKTIVITAS MENGGUNAKAN METODE REGRESI MLR DAN PCR

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INTISARI

Desain senyawa antikanker turunan benzoilhidrazon telah dilakukan melalui pendekatan analisis Hubungan Kuantitatif Struktur Aktivitas (HKSA) terhadap 30 senyawa turunan benzoilhidrazon menggunakan deskriptor hasil perhitungan metode DFT. Penelitian ini bertujuan untuk menentukan persamaan HKSA menggunakan metode regresi MLR dan PCR serta mendesain senyawa baru yang memiliki nilai aktivitas antikanker yang lebih tinggi berdasarkan persamaan HKSA yang telah diperoleh.

Hasil penelitian menunjukkan bahwa persamaan HKSA terbaik yang diperoleh melalui metode MLR yaitu pIC_{50} = -172,86 + (qC1 × 1098,72) + (qC4 × 3347,39) + (qC5 × -13792,61) + (qC6 × 12338,40) + (qC7 × -3270,61) + (qC10 × -1138,13) + (qC11 × 24,71) + (qN1 × 314,59) + (qN2 × 71,76) + (E Lumo × 53,60) + (Log P × 0,73) + (P × -0,33) + (MW × 0,02) dengan parameter statistika yaitu n = 13, r^2 = 0,885, SEE = 0,315, F_{hitung}/F_{tabel} = 2,413 dan PRESS = 0,97. Sedangkan, persamaan HKSA terbaik yang diperoleh melalui metode PCR yakni pIC_{50} = -1,30 + (L1 × -0,31) + (L2 × 0,07) + (L3 × -0,04) dengan parameter statistika yaitu n = 3, r^2 = 0,332, SEE = 0,522, F_{hitung}/F_{tabel} = 1,151 dan PRESS = 5,187.

Desain senyawa baru dilakukan berdasarkan persamaan HKSA terbaik, melalui metode MLR. Senyawa (E)-N-(3-bromobenziliden)-4-isopropilbenzohidrazid merupakan desain senyawa baru yang memiliki nilai aktivitas antikanker IC_{50} terbaik sebesar 0.05 µM.

Kata kunci: antikanker, benzoilhidrazon, DFT, HKSA, MLR, PCR.

DESIGN OF ANTICANCER COMPOUND OF BENZOYLHYDRAZONE DERIVATIVES BASED ON QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP ANALYSIS USING MLR AND PCR REGRESSION METHODS

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ABSTRACT

The design of anticancer compounds of benzoylhydrazone derivatives has been carried out based on Quantitative Structure Activity Relationship analysis of 30 benzoylhydrazone derivatives using descriptors calculated by the DFT method. This study aims to determine the QSAR equation using MLR and PCR regression methods and to design new compound that have higher anticancer activity values based on the QSAR equation that has been obtained.

The result showed that the best QSAR equation obtained through the MLR method is pIC_{50} = -172.86 + (qC1 × 1098.72) + (qC4 × 3347.39) + (qC5 × -13792.61) + (qC6 × 12338.40) + (qC7 × -3270.61) + (qC10 × -1138.13) + (qC11 × 24.71) + (qN1 × 314.59) + (qN2 × 71.76) + (E Lumo × 53.60) + (Log P × 0.73) + (P × -0.33) + (MW × 0.02) with statistical parameters, n = 13, R^2 = 0.885, SEE = 0.315, $F_{calculation}/F_{table}$ = 2.413 and PRESS = 0.97. While, the equation using the PCR method is pIC_{50} = -1.30 + (L1 × -0.31) + (L2 × 0.07) + (L3 × -0.04) with statistical parameters, n = 3, R^2 = 0.332, SEE = 0.522, $F_{calculation}/F_{table}$ = 1.151 and PRESS = 5.187.

The design of new compound was carried out based on the best QSAR equation, through the MLR method, the compound was (E)-N-(3-bromobenzylidene)-4-isopropylbenzohydrazide with IC_{50} of 0.05 µM

Keywords: anticancer, benzoylhydrazone, DFT, MLR, PCR, QSAR.