ANALISIS HUBUNGAN KUANTITATIF STRUKTUR DAN AKTIVITAS SENYAWA TURUNAN FLAVON SEBAGAI ANTIKANKER TERHADAP SEL HeLa

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INTISARI

Analisis hubungan kuantitatif struktur-aktivitas (HKSA) senyawa turunan flavon sebagai antikanker sel Hela telah dilakukan menggunakan pendekatan metode *Multilinear Regression* (MLR) dan *Principal Component Regression* (PCR). Tujuan penelitian ini adalah mengkaji hubungan aktivitas antikanker dan deskriptor teoritik turunan senyawa flavon menggunakan metode MLR dan PCR. Deskriptor teoritik yang digunakan berupa parameter-parameter elektronik, sterik, dan lipofilitas yang dianalisis pada struktur hasil optimasi menggunakan metode DFT/B3LYP/6-311G. Analisis statistik dilakukan dengan menggunakan metode MLR dan PCR. Hasil analisis HKSA dari metode statistik sebagai berikut :

MLR : Deskriptor = 10 ; n = 18 ; R = 0,896 ; R^2 = 0,803 ; F_{hit} / F_{tab} = 1,061 ;
$PRESS_{int}$ = 0,156 ; $PRESS_{eks}$ = 0,166 ; SD = 0,118

PCR : Deskriptor = 3 ; n = 18; R = 0,697; R^2 = 0,486; F_{hit} / F_{tab} = 1,321;
$PRESS_{int}$ = 0,536; $PRESS_{eks}$ = 0,182; SD = 0,182

Dari hasil kajian direkomendasikan senyawa antikanker hipotesis baru yang memiliki aktivitas relatif baik berupa senyawa 6-[2-hidroksiiminoetoksi-2-(4-etoksifenil)etoksi] flavon.

Kata kunci : HKSA, flavon, regresi multilinier, regresi komponen utama.

ANALYSIS OF QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP OF FLAVONE DERIVATES AS ANTICANCER AGAINST HeLa CELL

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ABSTRACT

Quantitative structure-activity relationship (QSAR) analysis of flavon derivates compounds as anticancer against HeLa cell have been performed using multilinear regression (MLR) and principal component regression (PCR) analysis. The aim of this research was to investigate the relationship between anticancer activity and theoretical descriptors of flavon derivates using MLR and PCR methods. The theoretical descriptors that were used such as electronic, steric, and lipofility parameters which were analyzed from the optimized geometry structure performed by using DFT B3LYP 6-311G method. Statistical analysis were carried out using MLR dan PCR. The result of QSAR analysis from the statistical method were :

MLR : Descriptors = 10 ; n = 18 ; R = 0.896 ; R^2 = 0.803 ; F_{cal} / F_{tab} = 1.061 ;
$PRESS_{int}$ = 0.156 ; $PRESS_{ext}$ = 0.166 ; SD = 0.118

PCR : Descriptors = 3 ; n = 18 ; R = 0.697 ; R^2 = 0.486 ; F_{cal} / F_{tab} = 1.321 ;
$PRESS_{int}$ = 0.536 ; $PRESS_{ext}$ = 0.182 ; SD = 0,182

Based on the obtained equation, 6-[2-hydroxyiminoethoxy-2-(4-ethoxyphenyl) ethoxy]flavone compound has been recomended as hypothesis design of new anticancer that have relatively good activity.

Keywords : QSAR, flavone, multilinear regression, principal component regression.