QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP STUDY OF CURCUMIN ANALOGUES AS ANTI-PROLIFERATIVE AGENTS OF HUMAN PROSTATE CANCER CELL LINE (PC-3)

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ABSTRACT

A computational method for the Quantitative Structure-Activity Relationship Study of Curcumin Analogues as Anti-Proliferative Agents of Human Prostate Cancer Cell Line (PC-3) has been developed. The aims of this research were obtaining the best QSAR equation to find the relationship between anti prostate activity and the quantitative structure of curcumin derivative compounds and also designing new anti-prostate compounds from curcumin derivatives that have higher predictions based on the obtained QSAR equations.

Computational method validation and its basis set were carried out to find the best QSAR method that used to calculate electronic and molecular descriptors of curcumin derivatives. The QSAR equation was used to making the multilinear regression and making new compound from designing.

The results showed QSAR equation that had a good result on the model 1, namely pIC50=-4.489+(3.205xQC2) + (6.233XQC3) + (-7.214xQC4) + (-1.790xQC5) + (0.005xSurface Area (Grid)) and the obtaining QSAR equation can be model the new molecule and the result of the new modelling molecule had good IC_{50} which was below one, namely 0.82. The name of proposed molecule was (1E, 6E)- 7-(2,4-bis(dimethylamino)phenyl)-1-(2,3-dimercaptophenyl)-5-hydroxy-4-((trifluoromethyl)sulfonyl) hepta-1,6-dien-3-one.

Keywords: curcumin, prostate, QSAR

HUBUNGAN KUANTITATIF STRUKTUR AKTIVITAS ANALOG KURKUMIN SEBAGAI AGEN ANTI-PROLIFERASI PADA GARIS SEL KANKER PROSTAT MANUSIA (PC-3)

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INTISARI

Telah dikembangkan metode komputasi Hubungan Kuantitatif Struktur Aktivitas Analog Kurkumin sebagai Agen Anti-Proliferasi pada Garis Sel Kanker Prostat Manusia (PC-3). Penelitian ini bertujuan untuk mendapatkan persamaan HKSA terbaik untuk mengetahui hubungan aktivitas anti prostat dengan struktur kuantitatif senyawa turunan kurkumin serta merancang senyawa anti prostat baru dari turunan kurkumin yang memiliki prediksi lebih tinggi berdasarkan persamaan HKSA yang diperoleh.

Validasi metode komputasi dan basis setnya dilakukan untuk menemukan metode HKSA terbaik yang digunakan untuk menghitung deskriptor elektronik dan molekuler turunan kurkumin. Persamaan HKSA digunakan untuk membuat regresi multilinear dan membuat senyawa baru dari perancangan.

Hasil penelitian menunjukkan persamaan HKSA memiliki hasil yang baik pada model 1 yaitu pIC50=-4.489+(3.205xQC2) + (6.233XQC3) + (-7.214xQC4) + (-1.790xQC5) + (0.005x Luas Permukaan (Grid)) dan persamaan HKSA yang diperoleh dapat memodelkan molekul baru tersebut dan hasil pemodelan molekul baru mempunyai IC_{50} yang baik yaitu dibawah satu yaitu 0,82. Nama molekul yang diajukan adalah (1E, 6E)- 7-(2,4-bis(dimethylamino)phenyl)-1-(2,3-dimercaptophenyl)-5-hydroxy-4-((trifluoromethyl)sulfonyl) hepta-1,6-dien-3-one.

Kata kunci: kurkumin, prostat, HKSA