ABSTRACT

Quantitative Structure-Cytotoxic Activity Relationship of *N*-benzoyl-*N*'-(4-fluorophenyl)thiourea and its derivatives on MCF-7 Cell Line

In this study, we have done some initial step (docking, synthesis, cytotoxic assay, and QSAR) to develop one of thiourea derivatives, *N*-benzoyl-*N*'-(4-fluorophenyl)thiourea (FFTU), as a potential anticancer compound. First, FFTUs have been docked in a SirT1 receptor with PDB ID: 4I5I using MVD v5.5, then it showed that rerank score FFTUs were lower than Hydroxyurea (HU). It was predicted that FFTU has higher biological activity. Second, FFTUs were synthesized by two-step reaction between ammonium thiocyanate and benzoyl chloride derivatives then with 4-fluoroaniline. The structures of compounds were characterized by UV, IR,^{1}HNMR,^{13} CNMR, and Mass Spectrometer. third, the new compounds were screened for in vitro cytotoxic activity against MCF-7 cell line. Last, QSAR analysis between lipophilic, electronic, and steric parametric of substituent and whole molecule has been done. Result, there was a quantitative relationship between substituent parametric (π) and cytotoxic activity in MCF-7 cell line and it was proved by this equation : Log 1/C = -0,204π+ 0,647(N=4, r= 0,957, p= 0,043, F = 21,525, Se= 0,07652)

Keyword: in silico, anticancer, cytotoxic activity, QSAR, *N*-benzoyl-*N*'-(4-fluorophenyl)thiourea, MCF-7