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Molecular Modeling Studies on Series of A-Aminoacid Functionalized 4-Quinazoline Derivatives Based on Cytotoxic Activity Data Against U 937 Cell Lines

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ABSTRACT

*In continuation of our efforts on synthesis and in vitro anticancer activity evaluation against U937 cell lines of series of 2-phenyl-6-substituted quinazolin-4-yl amino acetic acid derivatives **6a-6o**, the data was compared with structure–based investigations using Docking studies with the crystal structure of caspase-1 protein (1BMQ). The binding energies estimated by scoring functions were found to have a good correlation with the experimental inhibitory potencies.*

Keywords: Cytotoxic activity; amino acids; quinazolines; cell lines; modeling studies.