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Data Article

Synthesis, DFT computations, molecular docking studies and anticancer activity of 2-(4-fluorophenyl)-3-(5-methylisoxazol-3-yl)thiazolidin-4-one

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ABSTRACT

A hybrid molecule of isoxazole and thiazolidine-4-one, 2-(4-fluorophenyl)-3-(5-methylisoxazol-3-yl)thiazolidin-4-one (3) was synthesized and characterized unambiguously using ^{1}HNMR, 2D NMR, ^{13}CNMR, IR, and LCMS. The extensive molecular and electronic parameters for compound 3 were calculated by using the DFT/B3LYP/6–311++*G*(d,p) level. The target compound 3 was evaluated for in vitro anticancer activity against HeLa, MCF7, A549, and HEK293 cell lines. Molecular docking studies in the active site of EGFR revealed the key interactions of compound 3 and the insilico ADME properties were calculated using SwissADME.

Specifications Table

Subject area	Organic Chemistry, Medicinal Chemistry, Spectroscopy, Computational Chemistry
Compounds	2-(4-fluorophenyl)−3-(5-methylisoxazol-3-yl)thiazolidin-4-one
Data category	Spectral, synthesized, computational simulations
Data acquisition format	NMR, IR, Mass spectra
Data type	Analyzed
Procedure	The target compound 2-(4-fluorophenyl)−3-(5-methylisoxazol-3-yl)thiazolidin-4-one was synthesized, characterized by various techniques, and studied for anticancer activity
Data accessibility	Supplementary data enclosed with the online version of this article

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