Abstract

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Graph Theoretical analysis and in silico modeling and molecular dynamic studies of thiazole derivatives for the modulation of glucose metabolism in 3T3-L1 adipocytes

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Abstract

The glucose utilisation efficiency of 1-(2-((1-(dimethylamino)-2-(4-substituted phenyl)vinyl) (methyl) amino)-4-(trifluoromethyl)thiazol-5-yl)ethan-1-one derivatives in 3T3-L1 adipocytes was investigated in the following study. The thiazole and its derivatives were found to have a wide range of biological actions, including anti-diabetic efficacy. Various spectral analyzers were used to assess the synthesized analogs, and the findings of the characterizations were used to corroborate the properties of the synthesized analogs.Methodology: The mechanism underpinning that the glucose utilisation of thiazole derivatives was investigated using molecular docking with the chosen target, and in silico studies revealed a robust interaction between thiazole derivatives and AMPK binding sites. The synthesized thiazole analogs were tested for their in vitro cellular viability and glucose uptake on 3T3-L1 adipocytes based on the significant report of in silico screening. Findings: Intriguingly, 40 g of 3a, 3d, 3l 3b, 3i, and 3j had a cellular viability of 78.2 2.76 percent, with no cell death seen at lower concentrations. Furthermore, glucose consumption was found to be concentration dependent in 3T3-L1 adipocytes at various 3a, 3d, 3l 3b, 3i, and 3j concentrations. In comparison to Metformin (10 M) and Insulin (10 M), the results of 3a, 3d, 3l 3b, 3i, and 3j (40 g) on glucose utilisation demonstrated an outstanding result of 4.54 percent. Conclusion: The findings showed that 1-(2-((2-(1-methylphenyl)-1-(dimethylamino) vinyl) (methyl) amino)-4-(trifluoro methyl) thiazol-5-yl) ethenone (3a) derivative greatly improved glucose utilisation efficiency and protected cells from insulin resistance.

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Biography

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