An in silico ADMET, molecular docking study and microwave-assisted synthesis of new phosphorylated derivatives of thiazolidinedione as potential anti-diabetic agents

ABSTRACT

A series of new phosphorylated derivatives of thiazolidinedione was synthesized for the first time with high yields (92–96%) in short reaction time (7–15min) by the reaction of 4-{[(5E)-2,4-dioxo-1,3-thiazolidin-5-ylidene]methyl}phenyl ethyl phosphorochloridate with various heterocyclic amines by microwave irradiation technique under solvent-free condition. A study on in silico ADMET and molecular docking was performed for all the molecules to acquire an insight on drug likeliness behavior and also their ability to inhibit the enzyme, α-amylase. The molecules with momentous pharmacokinetic properties with substantial binding affinity were synthesized. The synthesized compounds were characterized spectroscopically to confirm their structure and then in vitro α-amylase inhibitory activity was also carried out for all the newly prepared compounds. The compounds 9b, 9e, 9f, and 9j reported the highest inhibition amongst the synthesized compounds. All the leftover compounds displayed modest to excellent inhibition in comparison with reference drug, Acarbose.