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Investigations into the anti-inflammatory and anti-diabetic activity of newly synthesized derivatives of 4AP2BOB utilizing DFT, molecular docking and spectroscopic characterization

M. Selvakumaran [a], Predhanekar Mohamed Imran [a,*], Attar Kubaib [a,*], Mohammad Azam [b], A. Aathif Basha [c], Saud I. Al-Resayes [b]

[a] Department of Chemistry, Islamiah College (Autonomous), Vaniyambadi - 635752, Tamilnadu, India[1]
[b] Department of Chemistry, College of Science, King Saud University, PO BOX 2455 Riyadh, 11451 Saudi Arabia
[c] Department of Physics, Islamiah College (Autonomous), Vaniyambadi - 635752, Tamilnadu, India[1]

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ABSTRACT

Utilizing cutting-edge spectroscopic techniques, including FT-IR, ^{1}H NMR and ^{13}C NMR, we created and thoroughly evaluated novel forms of Acetamidophenyl-2-(benzoyloxy) benzoate. This study is coupled with the reduction of COX1, COX2 and alpha-amylase which are associated with diabetes and inflammation and that have shown encouraging outcomes in laboratory studies. The molecular structures of the title compound, , its vibrational frequencies and corresponding vibrational assignments have been investigated experimentally. Additionally, over the cube files of the molecule, FMO and MEP analyses were performed. Further, *in-silico* ADME research on the newly developed compounds was also done. Finally, the molecular docking calculations and in-depth drug-likeness profiling were conducted according to empirical rules related to ADME to validate the conclusions and designate precise binding interactions. Considering the findings of the study, it has been established that these novel compounds offer a great deal of promise as potent therapeutic agents for managing inflammation and diabetes.

1. Introduction

Diabetes mellitus refers to an excessive flow of sweet urine. One characteristic of diabetes mellitus was hyperglycemia brought on by deficits in insulin production, activity, or both [1]. This metabolic disorder's chronic hyperglycemia [2] has been related to long-term damage, dysfunction and failure of several organs, including the heart, blood vessels, kidneys, eyes, nerves and neurological system. Inadequate insulin levels lead to hyperglycemia. In this situation, blood glucose levels increase to the point that it "spills over" into the urine. As a result, cells hunger because the entry of glucose-activated molecules into the cells is impeded. Excessive thirst and frequent urination are symptoms of hyperglycemia.

The chronic elevation of blood glucose levels in diabetes mellitus poses significant risks to various organs, causing progressive damage and increasing the likelihood of complications. It underscores the importance of managing blood glucose levels effectively through lifestyle modifications, medication and regular monitoring to mitigate the long-term impact on organ health and overall well-being.

NSAIDs are a class of drugs that reduce or eliminate erythema, oedema, high fever and pain brought on by various inflammatory triggers. Evidence shows that all NSAIDs' anti-inflammatory effects are primarily mediated via reducing prostaglandin synthesis [3], although NSAID's mechanism of action (MOA) has been widely investigated. The cyclooxygenase enzyme was first identified by Vane as the therapeutic target of NSAIDs in 1971, revealing that these anti-inflammatory medications restrict the generation of prostaglandins (PGs), which are involved in several physiological and pathological processes [4]. The detailed understanding of NSAIDs' mechanism of action, particularly in inhibiting prostaglandin synthesis through cyclooxygenase enzyme modulation, provides a foundation for the therapeutic use of these medications in managing inflammatory conditions. Recognizing the specific pathways through which NSAIDs exert their effects enhances our ability to tailor treatments for optimal efficacy and minimal side

* Corresponding authors.
E-mail addresses: imranpkm@gmail.com (P.M. Imran), attar.kubaib@gmail.com (A. Kubaib).
[1] Affiliated to Thiruvalluvar University, Serkadu, Vellore – 632115, Tamilnadu, India.

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