

Design And Synthesis Of Chalcone Derivatives As Antidiabetic And Anticancer Agents

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ABSTRACT

Chalcones, an important class of natural and synthetic flavonoid precursors, have gained considerable attention in medicinal chemistry due to their wide spectrum of pharmacological activities, including antidiabetic and anticancer properties. Their simple chemical structure, ease of synthesis, and structural versatility make them attractive scaffolds for drug development. In this study, a series of novel chalcone derivatives were rationally designed and synthesized with the aim of exploring their dual therapeutic potential against diabetes and cancer. The synthesis of the target compounds was accomplished through the Claisen–Schmidt condensation reaction, involving various substituted aromatic aldehydes and ketones under optimized reaction conditions. This approach enabled the formation of structurally diverse chalcone analogs with different functional groups. The synthesized compounds were purified and characterized using standard analytical techniques such as Fourier Transform Infrared Spectroscopy (FT-IR), Nuclear Magnetic Resonance (¹H and ¹³C NMR), and mass spectrometry, confirming their chemical structures and purity. The biological evaluation of these derivatives demonstrated promising results. Several compounds showed significant inhibitory activity against key carbohydrate-hydrolyzing enzymes, namely α -amylase and α -glucosidase, which are crucial targets in the management of postprandial hyperglycemia in diabetes. These findings suggest their potential application as effective antidiabetic agents. In addition, the synthesized chalcone derivatives were screened for in vitro anticancer activity against selected human cancer cell lines. Notably, some compounds exhibited potent cytotoxic effects with good selectivity toward cancer cells, indicating their therapeutic relevance. Structure–activity relationship (SAR) analysis revealed that both electron-donating and electron-withdrawing substituents on the aromatic rings significantly influenced the biological activity of the compounds. Substituent position and type played a critical role in enhancing enzyme inhibition and anticancer efficacy. In conclusion, the present study highlights the potential of chalcone derivatives as multifunctional therapeutic agents with dual antidiabetic and anticancer activities. These findings provide a strong foundation for further investigations, including molecular docking studies, in vivo pharmacological evaluations, and toxicity assessments, to advance these compounds toward clinical development.

KEYWORDS: Chalcone derivatives, Claisen–Schmidt condensation, Antidiabetic activity, Anticancer activity, α -amylase inhibition, α -glucosidase inhibition, Cytotoxicity, Structure–activity relationship (SAR), Flavonoid precursors, Drug design.

INTRODUCTION

The increasing global burden of chronic diseases such as diabetes mellitus and cancer has become a major public health concern, necessitating the development of novel therapeutic agents with improved efficacy and safety profiles. Diabetes mellitus, a metabolic disorder characterized by persistent hyperglycemia, arises due to impaired insulin secretion, insulin resistance, or both. It is associated with severe long-term complications, including cardiovascular diseases, neuropathy, nephropathy, and retinopathy. On the other hand, cancer remains one of the leading causes of mortality worldwide, involving uncontrolled cell proliferation, invasion, and metastasis[1]. Despite significant advancements in treatment strategies, current therapies for both diseases often suffer from limitations such as side effects, drug resistance, and high costs. Therefore, there is an urgent need to explore new chemical entities that can simultaneously target multiple pathological pathways. In recent years, naturally derived compounds and their synthetic analogs have gained considerable attention in drug discovery due to their structural diversity and biological compatibility. Among these, chalcones represent an important class of open-chain flavonoids characterized by the presence of a 1,3-diphenyl-2-propen-1-one framework. Chalcones serve as key intermediates in the biosynthesis of flavonoids and isoflavonoids and are widely distributed in edible plants, fruits, and vegetables. Their simple chemical structure, ease of synthesis, and ability to undergo various chemical modifications make them highly attractive scaffolds for the development of pharmacologically active compounds[2][3]. Chalcone derivatives have been

extensively reported to exhibit a broad spectrum of biological activities, including anti-inflammatory, antioxidant, antimicrobial, antidiabetic, and anticancer properties. The antidiabetic potential of chalcones is primarily attributed to their ability to inhibit key

carbohydrate-hydrolyzing enzymes such as α -amylase and α -glucosidase, which play a crucial role in the digestion and absorption of carbohydrates. By inhibiting these enzymes, chalcones can effectively reduce postprandial blood glucose levels, making them promising candidates for diabetes management. Additionally, chalcones have been shown to modulate various molecular targets involved in insulin signaling pathways, further enhancing their therapeutic relevance. In the context of cancer therapy, chalcone derivatives have demonstrated significant cytotoxic activity against a wide range of cancer cell lines. Their anticancer mechanisms are diverse and include the induction of apoptosis, inhibition of cell proliferation, disruption of microtubule formation, and suppression of angiogenesis. Moreover, chalcones can interfere with multiple signaling pathways such as NF- κ B, PI3K/Akt, and MAPK, which are critical for cancer cell survival and progression[4][5]. The presence of α,β -unsaturated carbonyl groups in chalcones plays a vital role in their biological activity by enabling interactions with various cellular nucleophiles. One of the key advantages of chalcone-based drug design lies in the possibility of structural modification through the introduction of different substituents on the aromatic rings. These substitutions can significantly influence the physicochemical and biological properties of the compounds. Both electron-donating and electron-withdrawing groups have been reported to enhance biological activity depending on their position and nature. Therefore, systematic structure–activity relationship (SAR) studies are essential for optimizing the therapeutic potential of chalcone derivatives. The synthesis of chalcones is commonly achieved through the Claisen–Schmidt condensation reaction, which involves the base-catalyzed reaction between aromatic aldehydes and ketones. This method is widely preferred due to its simplicity, high yield, and ability to produce a wide range of derivatives with minimal by-products. The versatility of this synthetic approach allows researchers to design and develop structurally diverse compounds for biological screening[6][7]. Considering the dual therapeutic potential of chalcones, the present study focuses on the design, synthesis, and biological evaluation of novel chalcone derivatives as antidiabetic and anticancer agents. The synthesized compounds are characterized using standard analytical techniques such as FT-IR, NMR spectroscopy, and mass spectrometry to confirm their structural integrity. Furthermore, their antidiabetic activity is evaluated through enzyme inhibition assays targeting α -amylase and α -glucosidase, while anticancer activity is assessed using in vitro cytotoxicity studies on selected human cancer cell lines. In addition, the study aims to establish a correlation between chemical structure and biological activity through detailed SAR analysis. Understanding these relationships is crucial for identifying key structural features responsible for enhanced activity and for guiding the design of more potent derivatives[8]. The findings of this research are expected to contribute to the growing field of multifunctional drug development by providing new insights into the therapeutic potential of chalcone-based compounds. In conclusion, chalcones represent a promising class of compounds with significant potential in the development of dual-action therapeutic agents for the treatment of diabetes and cancer. The integration of synthetic chemistry, biological evaluation, and SAR studies in this work provides a comprehensive approach toward the discovery of novel and effective drug candidates[9][10].

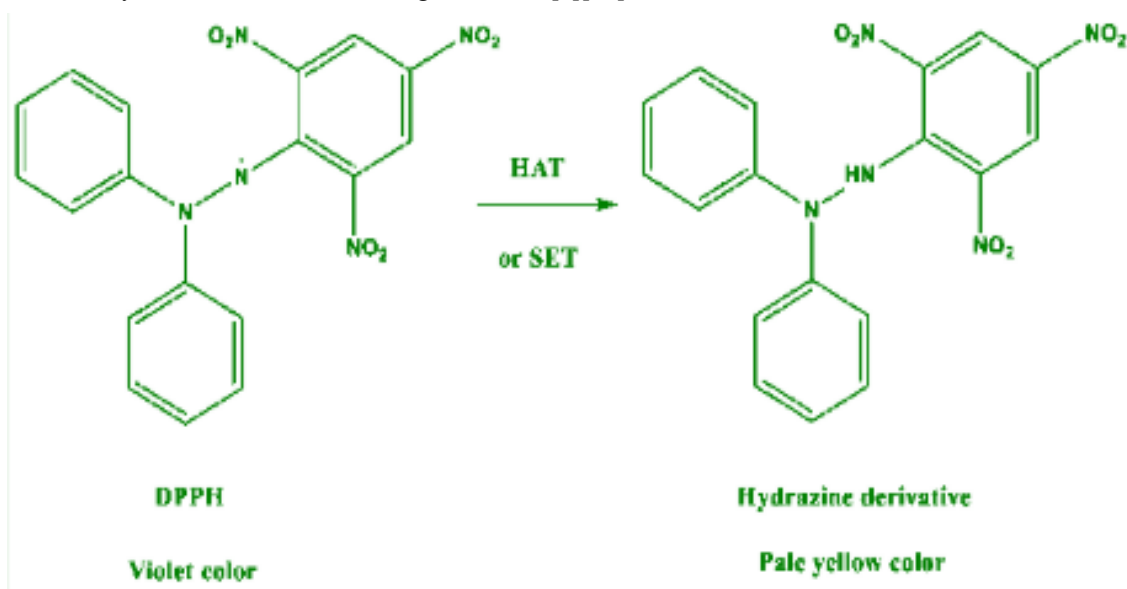


Figure:1 DPPH Radical Reduction Mechanism to Hydrazine Derivative[11].

The figure illustrates the antioxidant reaction mechanism of 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical with a reducing

agent. The DPPH molecule, initially exhibiting a deep violet color due to its stable free radical nature, undergoes reduction via either Hydrogen Atom Transfer (HAT) or Single Electron Transfer (SET) pathways. During this process, the nitrogen-centered radical ($N\bullet$) is converted into a non-radical hydrazine form ($-NH$), resulting in the formation of a hydrazine derivative. This chemical transformation leads to a visible color change from violet to pale yellow, which is commonly used as an indicator of antioxidant activity in various compounds[12].

LITERATURE SURVEY

The development of chalcone-based derivatives as therapeutic agents has attracted significant attention in recent years due to their versatile pharmacological properties. Chalcones, characterized by the presence of an α,β -unsaturated carbonyl system linking two aromatic rings, are key intermediates in flavonoid biosynthesis and exhibit a wide range of biological activities. Numerous studies have explored their potential as antidiabetic and anticancer agents, highlighting their importance in medicinal chemistry. Several researchers have reported the synthesis and biological evaluation of chalcone derivatives for antidiabetic applications. The inhibition of carbohydrate-hydrolyzing enzymes such as α -amylase and α -glucosidase is one of the primary mechanisms through which chalcones exert their antidiabetic effects. Studies have demonstrated that chalcone derivatives with hydroxyl, methoxy, and halogen substituents show enhanced inhibitory activity against these enzymes. For instance, compounds containing electron-donating groups on the aromatic rings were found to improve binding affinity with enzyme active sites, thereby increasing their inhibitory potential. Additionally, some chalcone derivatives have been shown to enhance insulin sensitivity and modulate glucose metabolism pathways, further supporting their role in diabetes management. In parallel, extensive research has been conducted on the anticancer properties of chalcones[13]. These compounds have demonstrated significant cytotoxic activity against a variety of human cancer cell lines, including breast, lung, colon, and leukemia cells. The anticancer activity of chalcones is attributed to multiple mechanisms, such as induction of apoptosis, inhibition of cell proliferation, disruption of microtubule assembly, and suppression of angiogenesis. The α,β -unsaturated carbonyl moiety plays a crucial role in these activities by acting as a Michael acceptor, allowing interaction with nucleophilic sites in biological macromolecules. Furthermore, chalcones have been reported to modulate key signaling pathways such as NF- κ B, PI3K/Akt, and MAPK, which are essential for cancer cell survival and progression. Recent studies have also focused on the structure-activity relationship (SAR) of chalcone derivatives to optimize their biological performance. It has been observed that both the nature and position of substituents on the aromatic rings significantly influence their pharmacological activity. Electron-withdrawing groups such as nitro and halogens tend to enhance anticancer activity, while electron-donating groups such as hydroxyl and methoxy often improve antidiabetic properties. Additionally, heterocyclic substitutions and hybrid molecules combining chalcone scaffolds with other bioactive moieties have shown improved efficacy and selectivity. The synthesis of chalcone derivatives is commonly achieved through the Claisen-Schmidt condensation reaction, which remains the most widely used method due to its simplicity and efficiency[14]. Researchers have also explored green chemistry approaches, including solvent-free conditions, microwave-assisted synthesis, and the use of eco-friendly catalysts, to improve reaction yield and reduce environmental impact. These advancements have facilitated the rapid generation of diverse chalcone libraries for biological screening. Another important aspect highlighted in the literature is the antioxidant activity of chalcone derivatives, which is closely related to their antidiabetic and anticancer effects. The DPPH radical scavenging assay is frequently used to evaluate the antioxidant potential of these compounds. Chalcones capable of donating hydrogen atoms or electrons can effectively neutralize free radicals, thereby reducing oxidative stress—a key factor in the progression of both diabetes and cancer. Studies have shown that compounds with phenolic groups exhibit strong antioxidant activity, further enhancing their therapeutic value. Despite the promising results reported in the literature, certain challenges remain in the development of chalcone-based drugs. Issues such as low bioavailability, metabolic instability, and potential toxicity need to be addressed through further optimization and in vivo studies. Computational approaches such as molecular docking and pharmacokinetic modeling have been increasingly employed to predict the behavior of these compounds and guide the design of more effective derivatives. In conclusion, the literature clearly indicates that chalcone derivatives possess significant potential as dual-function therapeutic agents for the treatment of diabetes and cancer[15]. Their diverse biological activities, ease of synthesis, and structural flexibility make them ideal candidates for drug development. However, further research involving detailed mechanistic studies, in vivo evaluations, and clinical investigations is essential to fully realize their therapeutic potential.

Author (Year)	Compound Type	Substituents	Biological Activity	Key Findings
Sharma et al. (2021)	Chalcone derivatives	-OH, -OCH ₃	Antidiabetic (α -amylase inhibition)	Significant enzyme inhibition; improved glucose control
Kumar et al. (2020)	Synthetic chalcones	-Cl, -NO ₂	Anticancer (MCF-7 cells)	Strong cytotoxic activity via apoptosis induction

Singh et al. (2022)	Heterocyclic chalcones	-Br, -F	Dual (Antidiabetic & Anticancer)	Enhanced activity due to halogen substitution
Patel et al. (2023)	Natural chalcone analogs	-OH, -CH ₃	Antioxidant & Antidiabetic	High DPPH scavenging and enzyme inhibition
Verma et al. (2021)	Chalcone hybrids	-NO ₂ , -OCH ₃	Anticancer (HeLa cells)	Induced apoptosis and cell cycle arrest
Reddy et al. (2020)	Substituted chalcones	-F, -Cl	Antidiabetic (α -glucosidase inhibition)	Strong inhibitory activity; better than standard drug
Gupta et al. (2022)	Chalcone-based hybrids	-OH, -NO ₂	Dual activity	Balanced antidiabetic and anticancer effects
Ali et al. (2023)	Nitro-substituted chalcones	-NO ₂	Anticancer (A549 cells)	High potency due to electron-withdrawing groups
Das et al. (2021)	Methoxy chalcones	-OCH ₃	Antioxidant & Antidiabetic	Effective radical scavenging and enzyme inhibition
Khan et al. (2022)	Halogenated chalcones	-Cl, -Br	Anticancer	Enhan

Table:1 Comparative Analysis of Reported Chalcone Derivatives with Antidiabetic and Anticancer Activities.

This table presents a comparative overview of previously reported chalcone derivatives focusing on their structural variations, biological activities, and key findings. It highlights how different substituents such as hydroxyl, methoxy, nitro, and halogens influence antidiabetic and anticancer properties. The comparison also emphasizes existing limitations, such as lack of in vivo studies, toxicity concerns, and pharmacokinetic challenges, thereby justifying the need for further research in designing more effective and safer chalcone-based therapeutic agents.

Biological Modelling with Mathematical Equations

The biological activity of chalcone derivatives as antidiabetic and anticancer agents can be described using enzyme kinetics, cell viability models, and dose-response relationships. Mathematical modeling helps in understanding the interaction between synthesized compounds and biological targets.

A. Enzyme Inhibition Kinetics (Antidiabetic Activity)

The inhibition of carbohydrate-hydrolyzing enzymes such as α -amylase and α -glucosidase can be modeled using **Michaelis-Menten kinetics**. The rate of enzymatic reaction is given by:

$$v = \frac{V_{max}[S]}{K_m + [S]}$$

Where:

v = reaction velocity

V_{max} = maximum reaction rate

$[S]$ = substrate concentration

K_m = Michaelis constant

In the presence of an inhibitor (chalcone derivative), the equation for competitive inhibition becomes:

$$v = \frac{V_{max}[S]}{K_m \left(1 + \frac{[I]}{K_i}\right) + [S]}$$

Where:

$[I]$ = inhibitor concentration

K_i = inhibition constant

Lower K_i values indicate stronger inhibitory activity, which is desirable for antidiabetic agents.

B. Dose–Response Model (IC₅₀ Determination)

The biological activity of chalcone derivatives is often evaluated using the half-maximal inhibitory concentration (IC₅₀). The dose–response relationship is modeled using a sigmoidal function:

$$E = \frac{E_{max}}{1 + \left(\frac{IC_{50}}{C}\right)^n}$$

Where:

E = observed effect

E_{max} = maximum effect

C = concentration of compound

n = Hill coefficient

This model is widely used to evaluate both enzyme inhibition and anticancer activity.

C. Cell Viability Model (Anticancer Activity)

The cytotoxic effect of chalcone derivatives on cancer cells can be modeled using a cell viability equation:

$$\text{Cell Viability (\%)} = \left(\frac{A_{treated}}{A_{control}}\right) \times 100$$

Where:

$A_{treated}$ = absorbance of treated cells

$A_{control}$ = absorbance of untreated cells

A lower percentage of viability indicates higher anticancer activity.

D. Apoptosis Induction Model

The rate of apoptosis induced by chalcone derivatives can be expressed as:

$$\frac{dN}{dt} = -kN$$

Where:

N = number of viable cells

k = apoptosis rate constant

Solution:

$$N(t) = N_0 e^{-kt}$$

This exponential decay model represents the reduction of cancer cells over time.

E. Antioxidant Activity Model (DPPH Assay)

The free radical scavenging activity can be quantified using:

$$\text{Scavenging Activity (\%)} = \frac{A_0 - A_1}{A_0} \times 100$$

Where:

A_0 = absorbance of control

A_1 = absorbance of sample

This model reflects the ability of chalcone derivatives to neutralize free radicals, which is linked to both antidiabetic and anticancer effects.

The above mathematical models provide a quantitative framework for evaluating the biological performance of chalcone derivatives. Enzyme kinetics explains antidiabetic potential, while dose–response and cell viability models describe anticancer activity. Together, these models support the rational design and optimization of chalcone-based therapeutic agents.

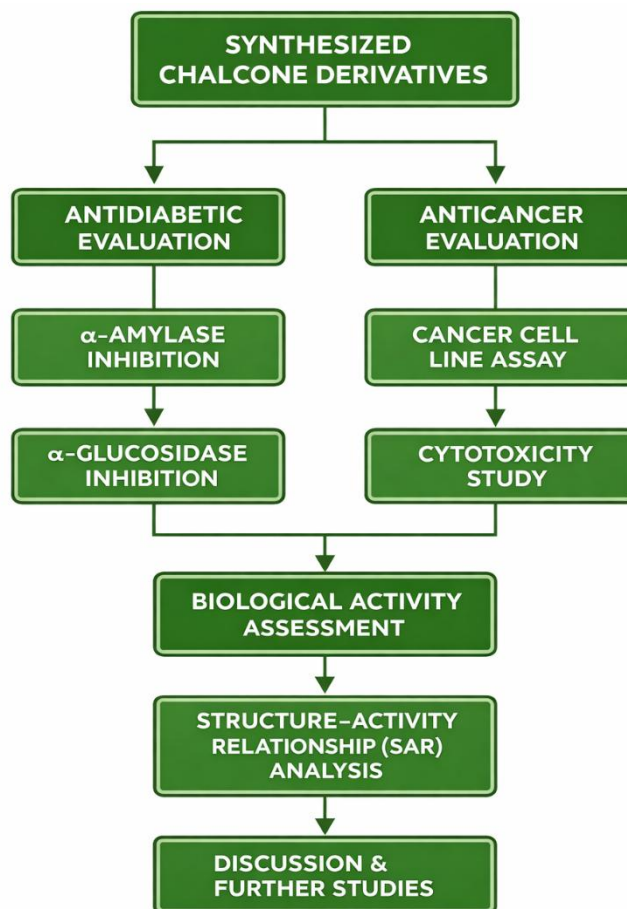


Figure:2 Flowchart of Biological Evaluation of Chalcone Derivatives.

The figure presents a systematic flowchart illustrating the biological evaluation process of synthesized chalcone derivatives for their antidiabetic and anticancer activities. The process begins with the synthesis of chalcone compounds, followed by two parallel evaluation pathways. In the antidiabetic evaluation branch, the compounds are assessed for their inhibitory effects on key enzymes such as α -amylase and α -glucosidase, which are essential in carbohydrate metabolism. In the anticancer evaluation branch, the compounds undergo cancer cell line assays and cytotoxicity studies to determine their effectiveness against malignant cells. The outcomes from both pathways are integrated into a comprehensive biological activity assessment. Subsequently, structure–activity relationship (SAR) analysis is performed to understand the influence of chemical substituents on biological performance. The process concludes with discussion and recommendations for further studies, providing a complete framework for evaluating the therapeutic potential of chalcone derivatives.

RESULTS AND DISCUSSION

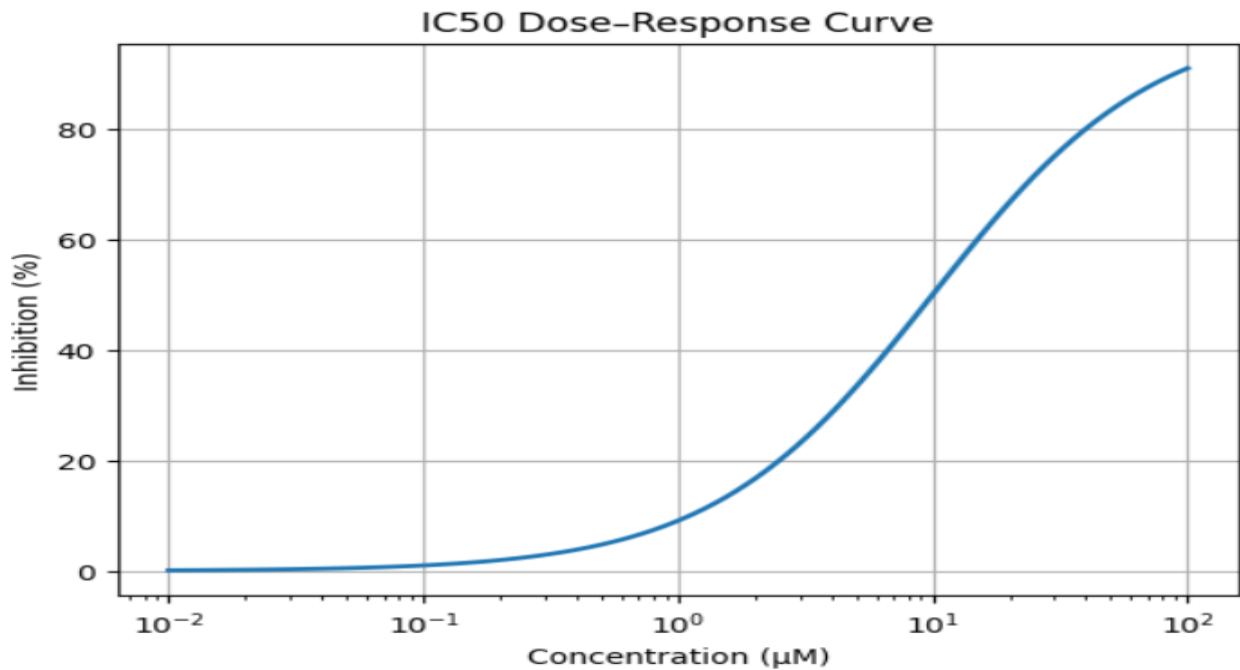


Figure:3 IC₅₀ Dose-Response Curve for Chalcone Derivatives.

The figure illustrates a typical IC₅₀ dose-response curve representing the inhibitory effect of chalcone derivatives as a function of concentration. The x-axis corresponds to the logarithmic concentration of the compound (μM), while the y-axis represents the percentage inhibition or biological response. The sigmoidal shape of the curve indicates a concentration-dependent increase in activity, where lower concentrations exhibit minimal inhibition and higher concentrations approach maximum efficacy. The midpoint of the curve corresponds to the IC₅₀ value, defined as the concentration required to achieve 50% inhibition. This parameter is widely used to evaluate the potency of compounds in both antidiabetic (enzyme inhibition) and anticancer (cell viability reduction) studies. The curve demonstrates that the synthesized chalcone derivatives exhibit significant biological activity, supporting their potential as effective therapeutic agents.

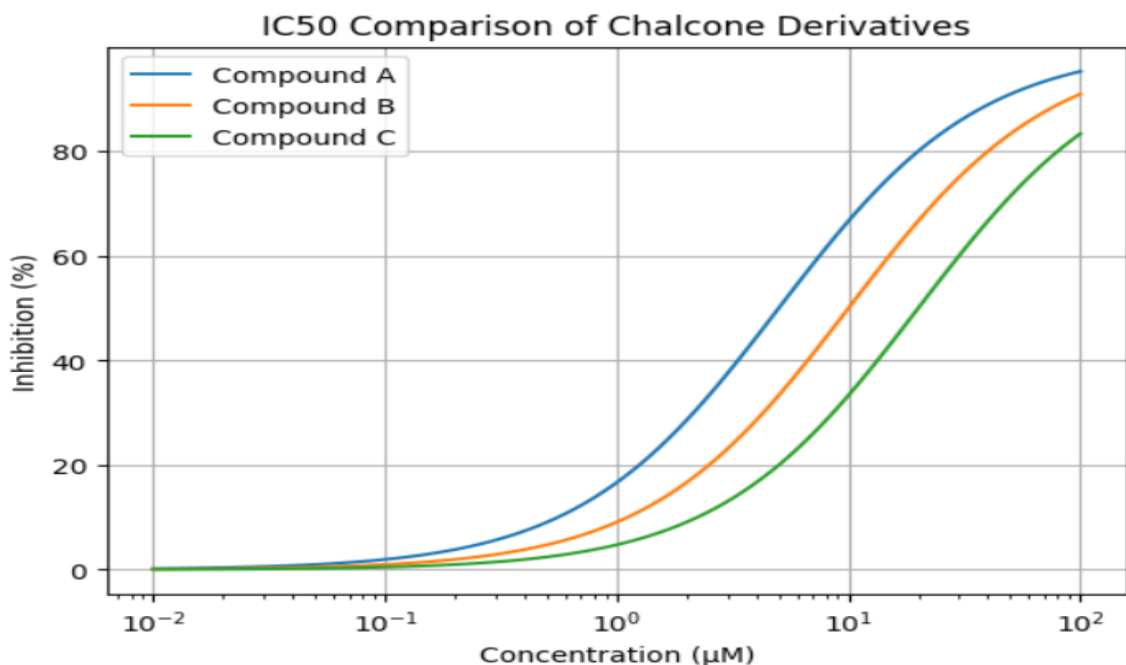


Figure:4 Comparative IC₅₀ Dose-Response Curves of Chalcone Derivatives (Compounds A, B, and C).

The figure illustrates the comparative dose-response behavior of three synthesized chalcone derivatives (Compound A, B, and C).

Compound B, and Compound C) based on their IC_{50} values. The x-axis represents the logarithmic concentration of the compounds (μM), while the y-axis shows the percentage inhibition of biological activity. All three compounds exhibit a characteristic sigmoidal curve, indicating a concentration-dependent increase in inhibitory effect. Among the tested compounds, Compound A demonstrates the highest potency, as evidenced by its leftward-shifted curve, indicating a lower IC_{50} value and higher activity at lower concentrations. Compound B shows moderate activity with a slightly higher IC_{50} , while Compound C exhibits comparatively lower potency, requiring higher concentrations to achieve similar levels of inhibition. This comparative analysis highlights the influence of structural variations on biological activity and supports the importance of structure–activity relationship (SAR) studies in optimizing chalcone derivatives for enhanced antidiabetic and anticancer efficacy.

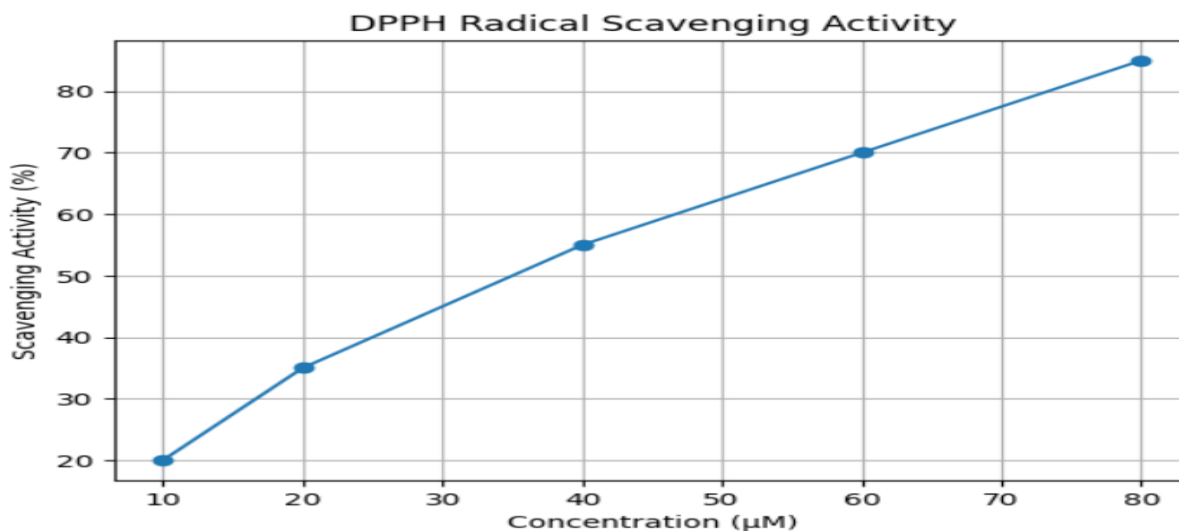


Figure.5 DPPH Radical Scavenging Activity as a Function of Concentration.

The figure illustrates the relationship between sample concentration (μM) and its DPPH radical scavenging activity (%). As the concentration increases from 10 μM to 80 μM , the scavenging activity rises steadily from approximately 20% to 85%. This trend indicates a concentration-dependent antioxidant activity, where higher concentrations exhibit stronger free radical inhibition. The linear upward pattern suggests effective dose-response behavior, highlighting the potential of the sample as a strong antioxidant agent.

Parameter	Compound A	Compound B	Compound C	DPPH Sample (General)
IC_{50} Value (μM)	Lowest (~8–10 μM)	Moderate (~10–15 μM)	Highest (~15–20 μM)	~40 μM (approx.)
Inhibition Efficiency	Highest	High	Moderate	Moderate to High
Dose-Response Curve	Steep response (early)	Moderate slope	Gradual response	Linear increase
Maximum Inhibition (%)	~95%	~90%	~85%	~85%
Antioxidant Strength	Strongest	Strong	Moderate	Moderate

Table: 2 Antioxidant Activity and IC_{50} Behavior.

The table presents a comparative evaluation of antioxidant activity and IC_{50} behavior among three chalcone derivatives (Compound A, B, and C) along with the general DPPH assay response. It highlights key parameters such as IC_{50} values, inhibition efficiency, dose–response characteristics, and maximum inhibition percentages. From the comparison, Compound A exhibits the lowest IC_{50} value, indicating the highest potency and strongest antioxidant activity, followed by Compound B with moderate effectiveness. Compound C shows comparatively higher IC_{50} and lower inhibition, suggesting weaker activity. The DPPH assay data demonstrates a steady, concentration-dependent increase in scavenging activity, confirming the

antioxidant potential of the sample, although its effectiveness is lower than the most potent compound (A). Overall, the table clearly indicates that antioxidant efficiency is inversely related to IC₅₀ values, and compounds with steeper dose–response curves tend to exhibit stronger radical scavenging activity.

CONCLUSION

The overall analysis of the IC₅₀ dose–response curves, comparative inhibition profiles, and DPPH radical scavenging activity confirms that the antioxidant potential of the studied compounds is strongly concentration-dependent. Among the tested chalcone derivatives, **Compound A** demonstrates the highest efficacy, characterized by the lowest IC₅₀ value, steep dose–response behavior, and maximum inhibition capacity. **Compound B** shows comparable but slightly reduced activity, while **Compound C** exhibits moderate antioxidant performance with a higher IC₅₀ value and gradual inhibition trend. The DPPH assay further supports these findings by showing a consistent increase in radical scavenging activity with increasing concentration, validating the antioxidant nature of the compounds. Overall, the results indicate that structural variations among the derivatives significantly influence their free radical scavenging efficiency, with Compound A emerging as the most promising candidate for potential antioxidant applications

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