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Spectral Characterization, ADME Prediction, and Antioxidant Activity of Chalcone Derivatives

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Abstract

Background: Oxidative stress, which happens when there are too many free radicals and not enough detoxification in the body, is linked to many long-term health problems.

Methods: In this research, a number of chalcone derivatives were synthesized, and their molecular structures were validated by infrared spectroscopy and other physicochemical analyses. We used computer programs to look at their pharmacokinetic behavior and see how they might be absorbed and metabolized in the body. We used a DPPH radical scavenging assay to test the antioxidant powers in a lab setting.

Results: Four chalcone derivatives (**B1**–**B4**) were efficiently synthesized with structural validation accomplished using FT-IR spectroscopy and physico-chemical characteristics. The SwissADME analysis verified advantageous pharmacokinetic characteristics and drug-likeness for every derivative. The DPPH radical scavenging assay indicated that all synthesized chalcone derivatives demonstrated robust antioxidant activity similar to the positive control ascorbic acid, establishing the chalcone scaffold as an efficient antioxidant pharmacophore.

Conclusion: Four chalcone derivatives (**B1**-**B4**) were successfully synthesized via the environmentally favorable Claisen-Schmidt condensation method. The drug-likeness criteria were met based on their ADME profiles, and they demonstrated substantial antioxidant activity comparable to that of standard ascorbic acid in DPPH radical scavenging assays. In medicinal chemistry, these compounds were identified as synthetic scaffolds with potential for enhancement and development into antioxidant agents for future therapeutic applications

التوصيف الطيفي، وتوقع حركيات الادوية، والنشاط المضاد للأكسدة لمشتقات الكالكون

مصطفى محمد حسين محمود

الخلاصة

المقدمة: يرتبط الإجهاد التأكسدي، الذي يحدث عند وجود الكثير من الجذور الحرة وعدم كفاية إزالة السموم في الجسم، بالعديد من المشاكل الصحية طويلة الأمد.

طرق العمل: في هذا البحث، تم تصنيع عدد من مشتقات الجالكون، وتم التحقق من صحة بنيتها الجزيئية باستخدام التحليل الطيفي بالأشعة تحت الحمراء والتحليلات الفيزيائية والكيميائية الأخرى. استخدمنا برامج حاسوبية لدراسة سلوكها الدوائي الحركي ومعرفة كيفية امتصاصها واستقلابها في الجسم. استخدمنا اختبار إزالة الجذور الحرة DPPH لاختبار قوى مضادات الأكسدة في بيئة معملية.

النتائج: تم تصنيع أربع مشتقات من الجالكون (**B1-B4**) بكفاءة، وتم التحقق من صحتها الهيكلية باستخدام التحليل الطيفي بالأشعة تحت الحمراء بتقنية تحويل فورييه (FT-IR) والخصائص الفيزيائية والكيميائية. وقد أثبت تحليل SwissADME خصائص حركية دوائية مواتية وتشابهًا دوائيًا لكل مشتق. أشارت تجربة إزالة الجذور الحرة DPPH إلى أن جميع مشتقات الجالكون المُصنّعة أظهرت نشاطًا مضادًا للأكسدة قويًا يُشبه حمض الأسكوربيك المُحاكي، مما يُثبت أن هيكل الجالكون هو مركب كيميائي فعال مضاد للأكسدة.

الاستنتاج: تم بنجاح تصنيع أربع مشتقات من الجالكون (**B1-B4**) باستخدام طريقة تكثيف كلايسن-شميدت الصديقة للبيئة. وقد استُوفيت معايير تشابه الأدوية بناءً على خصائص ADME الخاصة بها، وأظهرت نشاطًا مضادًا للأكسدة قويًا يُضاهي نشاط حمض الأسكوربيك القياسي في تجارب إزالة الجذور الحرة DPPH. في الكيمياء الطبية، تم تحديد هذه المركبات كهياكل اصطناعية ذات إمكانية للتحسين والتطوير إلى عوامل مضادة للأكسدة لتطبيقات علاجية مستقبلية.

1. Introduction

Oxidative stress happens when cells and tissues make and store too many reactive oxygen species (ROS), which are byproducts that the body can't get rid of quickly enough. Reactive oxygen species (ROS) are frequently produced during the metabolic degradation of oxygen within the body, and they serve essential functions, including the facilitation of intercellular signaling. But environmental stressors like ultraviolet (UV) radiation, ionizing radiation, pollution, heavy metals, and xenobiotics like antineoplastic medicines can raise them a lot. These factors cause oxidative stress, which is an imbalance that hurts cells and tissues (Dash et al., 2025). Thus, a key focus of modern pharmacological research is to generate breakthrough antioxidant medicines. The goal is to produce compounds that can effectively neutralize harmful free radicals and restore a healthy redox balance in cells. In laboratory and clinical settings, these drugs have shown promise in reducing oxidative damage and improving outcomes in models of neurodegeneration, tissue injury, and metabolic diseases (Yang et al., 2024). Chalcones, a type of phenolic compound that comes from plants, is one of the many substances being looked into. They are interesting because they have different shapes and biological roles (Hofmann et al., 2016). An α,β-unsaturated carbonyl moiety joins two aromatic rings. Most of the time, this system is in the stable E configuration. As seen in nature, these rings often have functional groups like hydroxyl and methoxy. Chalcones are an extremely valuable scaffold in drug discovery since they are easy to make, can be used in many ways, and are simple to work with. They are known for their many health benefits, such as fighting cancer, fighting infections, and getting rid of free radicals (Batovska & Todorova, 2010; Singh et al., 2014). This paper elucidates the synthesis of a series of chalcone derivatives via Claisen-Schmidt condensation, employing Na_2CO_3 as a catalyst in aqueous solution, resulting in substantial quantities of the produced derivatives. We used infrared spectroscopy and a few other physical and chemical tests to make sure that all of the new chalcones have the right structures. We looked at their pharmacokinetic properties on the SwissADME platform to see if they could be used as drugs. This included figuring out important ADME factors, like bioavailability. Ultimately, we performed a conventional DPPH radical scavenging experiment to evaluate their efficiency as antioxidants.

2. Materials and Methods

2.1. Materials

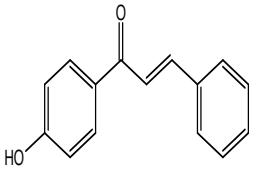
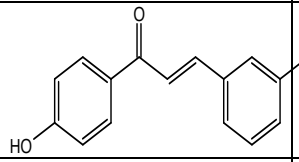
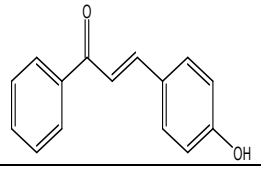
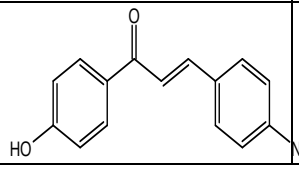
All chemicals were used without further purification and purchased from commercial sources, including p-hydroxy acetophenone, acetophenone, benzaldehyde, m-nitrobenzaldehyde, p-dimethylaminobenzaldehyde, and p-hydroxybenzaldehyde, were sourced from HiMedia (India), while 2,2-diphenyl-1-picrylhydrazyl (DPPH) was procured from Sigma-Aldrich (Germany). The melting points of all synthesized derivatives were measured via the open capillary method with a Stuart melting point apparatus (Stuart, England) and reported in their uncorrected form. Fourier-transform infrared (FT-IR) spectra were recorded on a Shimadzu

FT-IR 8400 spectrophotometer (Japan) using the potassium bromide (KBr) pellet technique at the Faculty of Pharmacy, University of Kufa. Reaction progress and the purity of products were regularly checked by ascending thin-layer chromatography (TLC) on Kieselgel GF254 aluminum plates (60 mesh, E. Merck, Germany), employing a solvent mixture of petroleum ether (40–60°C) and ethyl acetate (70:30 v/v) for elution, with spot visualization achieved through iodine vapor, UV light (254 nm), or appropriate derivatization. The DPPH assay was performed using a TECAN microplate reader (Austria), and all incubations took place in a temperature-controlled Infitek heating incubator (China).

2.2. ADMET Properties Analysis

The SwissADME online tool was employed to comprehensively predict the absorption, distribution, metabolism, and excretion (ADME) profiles of the designed chalcone derivatives (**B1**-**B4**), alongside critical pharmacokinetic parameters such as blood-brain barrier permeability, P-glycoprotein (P-gp) substrate recognition, and overall drug-likeness. Early drug discovery benefits greatly from this *in silico* platform, which makes it possible to identify promising candidates with excellent pharmacokinetic properties and effectively weed out compounds that are more likely to fail in later stages of development because of suboptimal ADME characteristics (Daina et al., 2017), Table1.

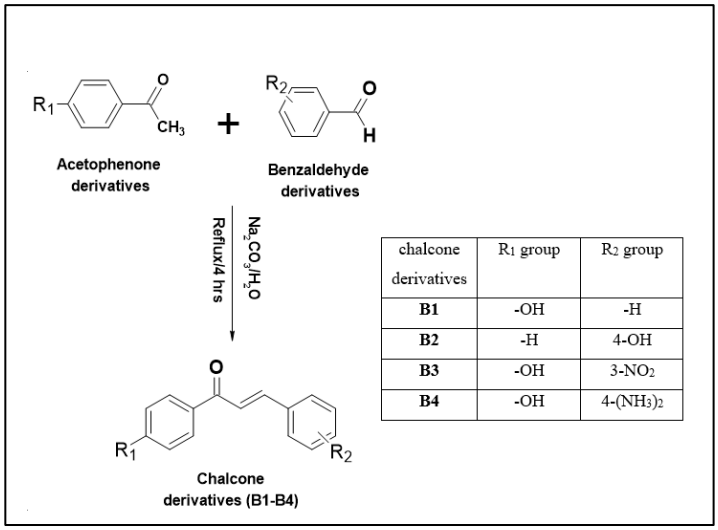
Table1: The molecular structures and their SMILEs of the designed chalcone derivatives (**B1**-**B4**).

Comp.	IUPAC name	Molecular Structure	SMILEs
B1	(E)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one		OC1=CC=C(C(/C=C/C2=CC=CC=C2)=O)C=C1
B2	(E)-3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one		O=C(/C=C/C1=CC=C(O)C=C1)C2=CC=CC=C2
B3	(E)-1-(4-hydroxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one		O=C(/C=C/C1=CC=CC([N+]([O-])=O)=C1)C2=CC=C(O)C=C2
B4	(E)-3-(4-(dimethylamino)phenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one		O=C(/C=C/C1=CC=C(N(C)C)C=C1)C2=CC=C(O)C=C2

2.3. Chemical synthesis

2.3.1. General Procedure for the Synthesis of Chalcone Derivatives (B1-B4)

Chalcone derivatives **B1**-**B4** were synthesized via Claisen-Schmidt condensation using equimolar quantities (10 mmol) of appropriate precursors: p-hydroxyacetophenone with benzaldehyde, m-nitrobenzaldehyde, or p-dimethylaminobenzaldehyde, and acetophenone with p-hydroxybenzaldehyde. The reactants were dissolved in deionized water (20 ml) under vigorous stirring in a preheated oil bath. Aqueous sodium carbonate solution (2.5 mmol, 0.265 g in 5 ml water) was added dropwise, and the mixture was refluxed at 100°C for 4 hours with continuous magnetic stirring. Reaction progress was monitored by TLC. Upon completion, the mixture was cooled to room temperature, and the precipitated products were collected by Büchner filtration. The crude products were washed with distilled water (2 × 30 ml) and cold absolute ethanol (2 × 10 ml), then air-dried to afford analytically pure chalcone derivatives without further purification, as depicted in Fig.1 (Hasan et al., 2015). The purity of the products was confirmed through the use of thin layer chromatography (TLC) examination as well as melting point determination. The completion of the structural confirmation was made possible through the evaluation of physicochemical properties and FT-IR spectroscopy, as shown in Tables3 and 4.



chalcone derivatives	R_1 group	R_2 group
B1	-OH	-H
B2	-H	4-OH
B3	-OH	3-NO_2
B4	-OH	4-$(NH_3)_2$

Figure1: Synthetic Diagram of The Chalcone Derivatives (B1-B4).

2.4. DPPH Assay

The radical-scavenging capacity of DPPH of the synthetic derivatives of chalcone (**B1**-**B4**) was evaluated using a standard procedure (Mensor et al., 2001). In this assay, methanolic solutions of each synthesized chalcone derivative and ascorbic acid, utilized as a positive control, were prepared at varying concentrations (62.5, 125, 250, and 500 µg/ml). Every sample solution was subsequently combined in a 1:1 ratio of volume with a fifty-microgram-per-milliliter solution of methanol containing DPPH. The resulting mixtures were

allowed to be incubated at 37°C for thirty minutes. Then the absorbance was spectrophotometrically measured at 517 nm using a reader on a microplate, with methanol as the blank. In order to guarantee both accuracy and reproducibility, all of the assays were carried out in triplicate. The following equation was utilized in the calculation of the percentage of activity that was exhibited by the scavenging of the DPPH radical:

$$\text{Radical scavenging (\%)} = [(\text{A})\text{control} - (\text{A})\text{sample}/\ (\text{A})\text{control}] \times 100$$

A curve of calibration was generated that showed the relationship between the percentage of scavenging activity for 2,2-diphenyl-1-picrylhydrazyl (DPPH) and concentration. The calibration curve was used to determine IC50 values.

2.5. Statistical and Mathematical Analysis

In the present investigation, Excel LTSC Professional Plus 2021 was used to calculate the half-inhibitory concentrations (IC50) values of the synthetic chalcone derivatives (**B1**-**B4**) and positive control in the DPPH experiment.

3. Results and Discussion

3.1. ADME Study Results

The pharmacokinetic properties of chalcone derivatives **B1**-**B4** were evaluated using the SwissADME computational platform Table2. All compounds demonstrated favorable drug-like characteristics with molecular weights ranging from 224.26 to 269.25 g/mol, well within Lipinski's rule of five criteria. The compounds exhibited optimal lipophilicity values (iLOGP: 2.45-3.45), indicating balanced hydrophilic-lipophilic properties suitable for membrane permeation. Notably, all derivatives showed high gastrointestinal absorption potential and blood-brain barrier permeability, suggesting excellent oral bioavailability and potential CNS activity. The topological polar surface area (TPSA) values varied significantly: **B1**, **B2**, and **B4** derivatives displayed low TPSA values (37.30-40.54 Å²), while **B3** derivative exhibited a higher value (83.12 Å²) due to the nitro group contribution. All TPSA values remained below the 140 Å² threshold for passive membrane permeability. Importantly, none of the compounds were predicted as P-glycoprotein substrates, minimizing efflux-mediated drug resistance potential. All derivatives achieved excellent bioavailability scores (0.85) and satisfied Lipinski's rule of five, confirming their drug-likeness. The identical ADME profiles of positional isomers **B1** and **B2** suggest that hydroxyl group location does not significantly influence pharmacokinetic properties. In contrast, substituent effects were evident, with the nitro group in **B3** derivative reducing lipophilicity (iLOGP = 2.45) while the dimethylamino group in **B4** derivative enhanced it (iLOGP = 3.45).

Table2: The Output Parameters of Drug-Likeness and ADME For the Designed Chalcone Derivatives (B1-B4) In the Swissadme Platform.

Parameters Comp.	MW (g/mol)	nRB	nHBA	nHBD	MR (m^3/mol)	TPSA (Å^2)	iLOGP	GI absorption	BBB permeant	P-gp	BS	Ro5
B1	224.26	3	2	1	67.89	37.30	2.89	High	Yes	No	0.85	Yes
B2	224.26	3	2	1	67.89	37.30	2.89	High	Yes	No	0.85	Yes
B3	269.25	3	4	1	73.42	83.12	2.45	High	Yes	No	0.85	Yes
B4	267.32	4	2	1	78.95	40.54	3.45	High	Yes	No	0.85	Yes

3.2. Chemical synthesis

Physicochemical and FT-IR spectral data for the chalcone derivatives (**B1-B4**) are given in Tables3 and Table4.

Table3: Physicochemical Data for The Synthesized Chalcone Derivatives (B1-B4).

Comp.	Physical appearance	Yield (%)	Melting point C^o	R_f
B1	Red solid	77	173-175	0.55
B2	Green solid	76	184-185	0.36
B3	Red solid	60	231-233	0.36
B4	Yellow solid	70	184-186	0.26

The Fourier Transform Infrared Spectra (FT-IR) analysis was employed to identify the specific absorbance bands of the synthesized chalcone derivatives (**B1-B4**), which are tabulated in Table4. Following the clarification of the absorbance bands, the functional groups in these derivatives were identified (Silverstein & Webster, 1996). All compounds exhibited distinctive carbonyl (C=O) stretching vibrations in the range of 1635-1651 cm^{-1}, confirming the presence of the α,β-unsaturated ketone moiety essential for chalcone structure. The trans C=C stretching appeared consistently at 1599-1606 cm^{-1}, indicating successful formation of the E-configuration double bond characteristic of chalcone derivatives. The phenolic hydroxyl (O-H) stretching was observed at varying frequencies: 3122 cm^{-1} (**B1**, **B4**), 3234 cm^{-1} (**B2**), and 3161 cm^{-1} (**B3**), reflecting different hydrogen bonding environments. Aromatic C-H stretching frequencies ranged from 3020 to 3066 cm^{-1}, confirming the presence of aromatic rings in all derivatives. Asymmetric C-O stretching vibrations appeared at 1217-1234 cm^{-1}, supporting the phenolic character. Derivative **B3** displayed additional characteristic peaks at 1556 and 1346 cm^{-1}, corresponding to asymmetric and symmetric N-O stretching of the nitro group, respectively. Derivative **B4** exhibited distinct methyl C-H stretching at 2970 and 2810 cm^{-1} (asymmetric and symmetric) and aromatic C-N stretching at 1348 cm^{-1}, confirming the presence of the dimethylamino substituent.

Table4: Spectral Data of The Synthesized Chalcone Derivatives (B1-B4).

Comp.	IR spectra frequency (cm^{-1}), KBr pellets
B1	3122 (O-H) str, 3066 (C-H) str (Aromatic), 1645 (C=O) str, 1604 (C=C) trans str, 1220 (C-O) asym str.
B2	3234 (O-H) str, 3020 Aromatic (C-H) str, 1649 (C=O) str, 1599 (C=C) trans str, 1217 (C-O) asym str.
B3	3161 (O-H) str, 3020 Aromatic (C-H) str, 1651 (C=O) str, 1606 (C=C) trans str, 1556, 1346 (N-O) asym & sym str of nitro group, 1226 (C-O) asym str.
B4	3122 (O-H) str, 3040 Aromatic (C-H) str, 2970, 2810 (C-H) asym & sym str vib of methyl group, 1635 (C=O) str, 1604 (C=C) trans str, 1348 Aromatic (C-N) str, 1234 (C-O) asym str.

3.3. DPPH Assay Results

The antioxidant potential of the synthesized chalcone derivatives (**B1**-**B4**) was evaluated using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay, with ascorbic acid serving as the positive control. The antioxidant activity was expressed as IC_{50} values, representing the concentration required to inhibit 50% of DPPH radical activity. The DPPH assay findings showed that the four synthesized chalcone derivatives displayed varying degrees of antioxidant activity Table5 and Fig.2. The derivative **B4**, including a 4-(dimethylamino) phenyl substituent, had the highest antioxidant activity with an IC_{50} value of 33.09 ± 2.51 µg/ml. Subsequently, compounds **B1** and **B2** exhibited comparable moderate antioxidant activity, with IC_{50} values of 52.36 ± 3.45 µg/ml and 54.62 ± 2.88 µg/ml, respectively. Derivative **B3**, containing the 3-nitrophenyl group, exhibited the lowest antioxidant activity among the investigated derivatives, with an IC_{50} value of 91.15 ± 4.33 µg/ml. The synthesized chalcone derivatives exhibited significantly decreased antioxidant activity compared to the reference standard ascorbic acid, which had an IC_{50} value of 4.66 ± 0.62 µg/ml. The data are presented as mean ± standard error, indicating that the experimental results are reproducible with high reliability.

Table5: Antioxidant Effect of The Synthesized Chalcone Derivatives (B1-B4) And Ascorbic Acid (Vit. C) In the DPPH Assay.

Chalcone derivative	IC_{50} (µg/ml), (DPPH) assay
B1	52.36 ± 3.45
B2	54.62 ± 2.88
B3	91.15 ± 4.33
B4	33.09 ± 2.51
Ascorbic acid (Vit. C)	4.66 ± 0.62

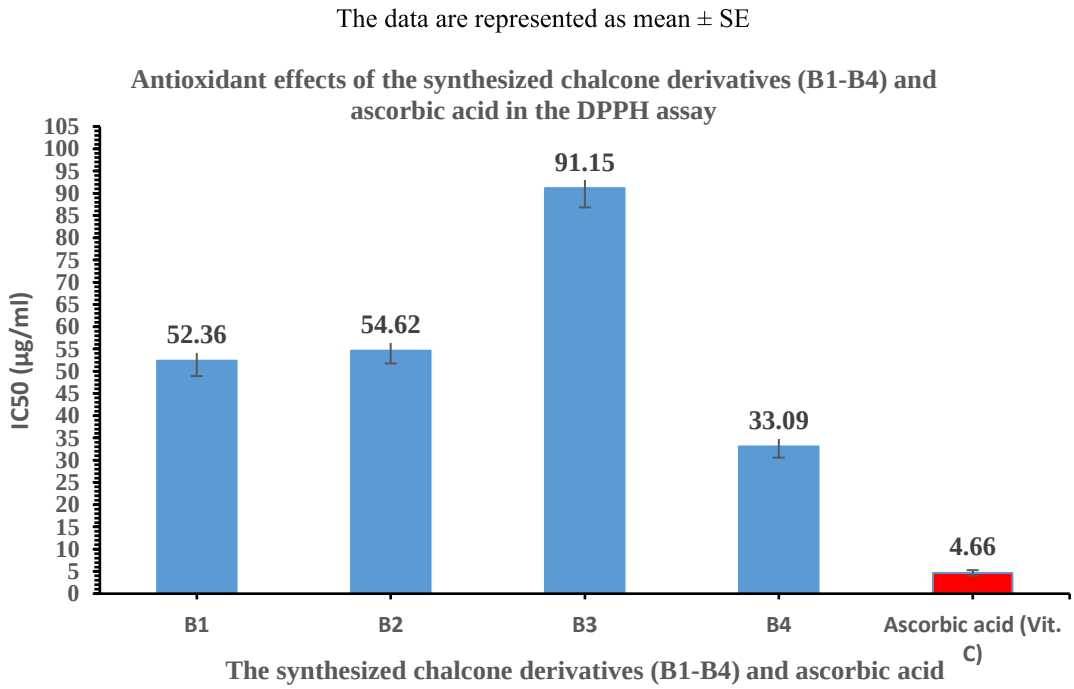


Figure1: Antioxidant Effect of The Synthesized Chalcone Derivatives (B1-B4) And Ascorbic Acid in The DPPH Assay.

Conclusion

The derivative **B4** showed the strongest antioxidant activity when compared to the other chalcone derivatives (**B1**-**B4**) that were synthesized in this work. Its IC_{50} value was 33.09 ± 2.51 µg/ml. The results of this study support the findings of previous research, which demonstrated that hydroxylated chalcone derivatives possess potent antioxidant properties. More specifically, structure-activity relationship analysis indicates that compounds containing electron-donating substituents, such as hydroxyl and dimethylamino groups, have enhanced abilities to scavenge radicals. Derivative **B4**, which contains a 4-(dimethylamino)phenyl substituent, has been found to have a higher level of effectiveness than other chemicals, which is evidence that aromatic structures that are rich in electrons assist in the process of radical neutralization by stabilizing resonance. This is the conclusion that can be drawn from the data. When substituents that pull electrons out of the molecule are applied, chalcone frameworks become less effective antioxidants (Hofmann et al., 2016; El-Atawy et al., 2024). Derivative **B3**, which has a 3-nitrophenyl group, has the least amount of antioxidant activity, with an IC_{50} value of 91.15 ± 4.33 micrograms per milliliter. Each of the synthesized chalcone

derivatives was found to comply with Lipinski's rule of five, which was determined utilizing the comprehensive ADME prediction study that was carried out on the SwissADME platform. The bioavailability of these compounds (0.85), their molecular weight (ranging from 224.26 to 269.25 g/mol), and their lipophilicity (iLOGP: 2.45-3.45) are all characteristics in which they are exceptionally proficient. Despite the fact that these drugs do not belong to the category of P-glycoprotein substrates, they all exhibit intriguing pharmacokinetic qualities that may be suitable for therapeutic applications. These features include their broad permeability across the blood-brain barrier as well as their high gastrointestinal absorption capacity. The computational predictions that have been made are in agreement with studies that have been carried out in recent times on chalcone derivatives. This agreement highlights the importance of the assessment of absorption, distribution, metabolism, and excretion (ADME) during the initial phases of drug discovery. This is due to the fact that drugs that have advantageous pharmacokinetic characteristics have increased therapeutic effectiveness in later biological tests. The hydroxyl and dimethylamino substituents that are present in this series maintain the justification for the methodology that was utilized in the development of the chalcone optimization techniques (Patil et al., 2024; Aydin et al., 2024) by maintaining drug-like properties as well as enhancing antioxidant activity. The findings shed some information on relationships between structure and activity, which could provide a basis for optimization studies that are conducted in the future. In addition to this, they provide evidence that demonstrates the possibility that chalcone derivatives (**B1**-**B4**) have the potential to be used as chemical scaffolds in the development of drugs that are effective antioxidants. The effective synthesis of a Claisen-Schmidt condensation that is environmentally friendly and employs a sodium carbonate catalyst serves to illustrate the practical accessibility of these molecules in the context of pharmaceutical research. Despite the fact that they are not as effective as ascorbic acid (IC_{50} = 4.66 ± 0.62 μg/ml) when it comes to their ability to act as antioxidants, the synthesized compounds are nevertheless deserving of additional exploration within the field of medicinal chemistry. This is owing to the good pharmacokinetic qualities and robust radical scavenging capabilities that they possess. If we want to increase the efficacy of antioxidants while at the same time maintaining the characteristics of drugs, then future research should concentrate on examining the incorporation of hydroxyl groups or other electron-donating substituents, which have shown potential in recent studies of chalcone derivatives that target diseases related to oxidative damage (Bułakowska et al., 2023).

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