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Acer Juma Hamad
Department of Chemistry, College of Science for Women, University of Baghdad, Baghdad, Iraq, aissar.awad2305m@csw.uobaghdad.edu.iq

Hamdia Hateem Jawad
Department of Chemistry, College of Science for Women, University of Baghdad, Baghdad, Iraq, Hamdiahateem@csw.uobaghdad.edu.iq

Kadhim A. Adem
Department of Physic, College of Science, University of Baghdad, Baghdad, Iraq, kadhim.aadim@sc.uobaghdad.edu.iq

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RESEARCH ARTICLE

Synthesis, Characterization, and Theoretical Investigation of the Effectiveness as Anti-corrosion for Chalcone Derivatives

Acer Juma Hamad [1,*], **Hamdia Hateem Jawad** [1], **Kadhim A. Adem** [2]

[1] Department of Chemistry, College of Science for Women, University of Baghdad, Baghdad, Iraq
[2] Department of Physic, College of Science, University of Baghdad, Baghdad, Iraq

ABSTRACT

In this research, the focus was on preparing a number of chalcone derivatives using the Claisen-Schmidt reaction method through the reaction of some benzaldehyde derivatives with acetophenone substitutes in the presence of a basic medium represented by (NaOH) at a concentration of 10%. The benzaldehyde derivatives and acetophenone derivatives were also dissolved in ethanol at a concentration of 98%. Before starting the preparation, a number of chalcone derivatives were banned, which were prepared and referred to as [Ch1, Ch2,Ch3, Ch4, Ch5]. The substitutes that were used in the preparation were 4-chlorobenzaldehyde, 4-aminoacetophenone, benzaldehyde, 3-Nitroacetophenone, 4-Nitrobenzaldehyde. Acetophenone,2-4-dichlorobenzaldehyde, and 4-(dimethylamino)benzaldehyde. The compounds were spectroscopically studied using FT-IR, 1H-NMR,13C NMR, and UV-Vis spectroscopy After that, the theoretical studies of the prepared compounds as corrosion inhibitors were conducted. They were studied theoretically using the Gaussian is a general purpose computational chemistry software package. Chalconate derivatives have the capacity to serve as electron donors as anti-corrosion agents. and it was found that derivative Ch5 is more effective theoretically as a corrosion inhibitor

Keywords: Chalcones derivatives, Characterization, Corrosion inhibition, Synthesis, Theoretical studies

Introduction

Chalcones, a prominent category of natural compounds, that fall within the flavonoid family, have been shown to exhibit several biological properties.[1,2] Chalcones are appropriate for the production of significant heterocycles such as indazole, cyclohexenone, isoxazoline, pyrimidine, and pyrazoline derivatives. Pyrazolines have garnered growing interest for their pharmacological uses, including their efficacy as antibacterial agents,[3] antifungal agents,[4] enzymatic inhibitors, and in the treatment of Parkinson's disease or head traumas.[5] Pyrazolines are utilized in the production of fluorescent dyes because of their optical characteristics.[6] In contrast, isoxazoline is recognized for its remarkable therapeutic capabilities in treating bacterial infections in both humans[7] and animals[8], as well as addressing immunological issues[9] and inhibiting tumor growth .Additionally, isoxazoline is employed as an insecticide, nematicide, and molluscicide.[10] Chalcone is a kind of organic compound that functions as both a ketone and an aldehyde, specifically an enone. Chalcone is known by several names, including benzylideneacetophenone, phenyl styryl ketone, benzalacetophenone, β-phenylacrylophenone, γ-oxo-α, γ-diphenyl-α-propylene, and α-phenyl-βbenzoylethylene.[11] The compound contains the ketoethylenic group (–CO–CH=CH-), Fig. 1

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* Corresponding Author.
E-mail addresses: aissar.awad2305m@csw.uobaghdad.edu.iq (A. J. Hamad), Hamdiahateem@csw.uobaghdad.edu.iq (H. H. Jawad), kadhim.aadim@sc.uobaghdad.edu.iq (K. A. Adem).

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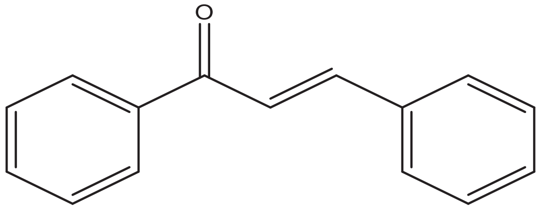


Fig. 1. Formula of chalcone.

There are several methods that may be used to prepare chalcones[12] Chalcones are typically produced by Claisen-Schmidt condensation performed in either a basic or acid environment, using homogenous conditions.[13] The Claisen Schmidt reaction has employed heterogeneous catalysts such as Lewis acids, Bronsted acids,or strong bases,with limited efficiency.[14] Many of them depend on the existence of certain catalysts The Claisen-Schmidt reactions for the synthesis of chalcones has been previously documented using particular catalysts,[15,16] as shown in Fig. 2.

Chalcones serve as initial substances for the production of other cyclic compounds,[17] such as pyrazolines and isoxazoles.Chalcone compounds have conjugated double bonds that are completely spread out across two aromatic rings, forming a π-electron system.[18]

The purpose of this research is to prepare chalcone derivatives, characterize them, and theoretically study their potential application as corrosion inhibitor compounds.[19]

Materials

The required chemical materials were obtained from CDH and BDH companies. Ethanol absolute with a purity of 99.7-100% was attained from Alpha Chemike company. Sodium hydroxide (NaOH) was acquired at a concentration of 10%. Other chemicals purchased include 4-chlorobenzaldehyde, 4-Aminoacetophenone, benzaldehyde, 3-Nitroacetophenone, 4-Nitrobenzaldehyde, acetophenone, 2-4-dichlorobenzaldehyde, and 4-(dimethylamino)benzaldehyde.

Methods

Method of Synthesis of Chalcones Derivative By Claisen_Schmidt[20] A mix of acetophenone substitutes (1.5 gm) or acetophenone (2 ml) was mixed with in 10 ml of ethanol, while benzaldehyde (2ml) was likewise dissolved in 10ml of ethanol. A 10% aqueous solution of NaOH (10 ml) was added to the mixture. The resulting solution was exposed to reflux for 2 hours on a magnetic stirrer, and then cooled in an ice bath for 12 hours. The precipitate was subjected to filters and then rinsed with ethanol and water.Recrystallization from 97% ethanol, filter it again, then leave it to dry, As shown in Fig. 3.

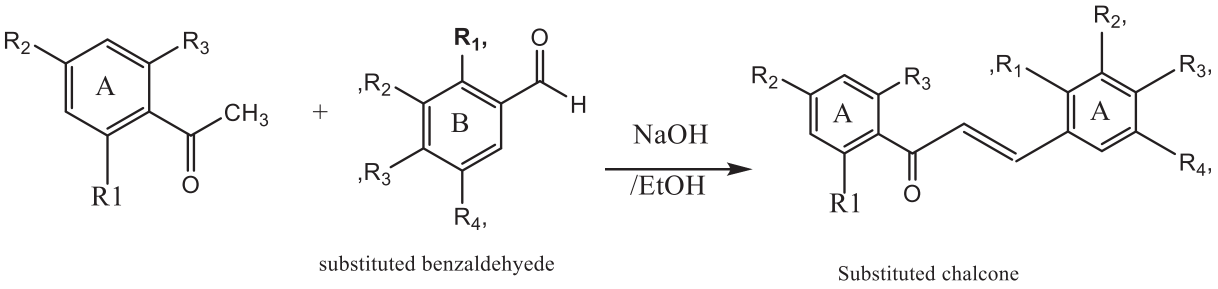


Fig. 2. Claisen _Schmidt condensation reaction in chalcones synthesis.

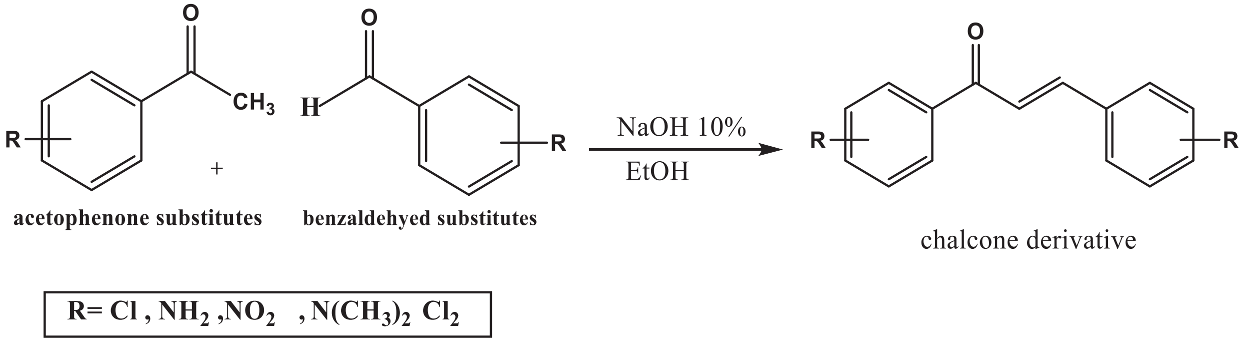


Fig. 3. Claisen _Schmidt condensation reaction in chalcones synthesis.

Table 1. Physical and analytical data of compounds.

No	M.F	M.W gm/ml	m.p.C^0	Colour
Ch1	$C_{15}H_{12}ClNO$	257.71 g/mol	93-95	Yellow
Ch2	$C_{15}H_{13}NO$	223.27 g/mol	106-108	Bright yellow
Ch3	$C_{15}H_{11}NO_3$	253.25 g/mol	130-132	Light brown
Ch4	$C_{15}H_{10}Cl_2O$	277.1 g/mol	71-73	Light yellow
Ch5	$C_{17}H_{16}N_2O_3$	296.32 g/mol	110-112	Dark brown

Instrumentation

All melting points were determined in open capillary tubes using a type device Gallen Kamp M.F.B-60. Infrared spectra were recorded with Shimadzu prestige-1800 FT-IR spectrometer using KBr discs. The 1H and 13C-NMR studies occurred at room temperature using a Bruker 400 MHz and Varian inova 500 MHz spectrometer, respectively, in DMSO-d6. The UV-Vis spectrum were obtained at room temperature using a UV-Visible The spectrophotometer is a Shimadzu UV-Vis 1900 model, operating within the wavelength range of 200 to 800 nm.

Study theory

The current research involves the use of the quantum program Gaussian 5.0. The Gauss View 5.0 package was utilized to determine the initial geometries of the chemical compounds. The calculations doing in Gas phase. In addition, using the B3LYP method, and using a basis set of 6.31G.[21]

Results and discussion

The Table 1 below presents the physical and analytical information for five chemical compounds, including their molecular formula, molecular weight, melting point, and color.

Molecular Weight (M.W.): The compounds have molecular weights that vary from 223.27 g/mol (Ch2) to 296.32 g/mol (Ch5). Ch5 has the highest molecular weight, whereas Ch2 has the lowest molecular weight. Molecular weight serves as a reliable measure of the magnitude and intricacy of a chemical substance.

Melting Point (M.P.): The melting points of compounds vary from 71-73 °C (Ch4) and 130-132 °C (Ch3). Ch3 exhibits the highest melting point, while Ch4 demonstrates the lowest melting point. The melting point is an indicator of the compound's thermal stability and the intermolecular interactions. The compounds exhibit a variety of hues, ranging from yellow to a deep shade of brown. The colors reflect changes in the compounds' molecular structure and bonding, influencing the way light absorbs and reflects.

It is worth mentioning that compounds with greater molecular weight generally exhibit higher melting temperatures, which suggests a more intricate structure and stronger chemical interactions. Nevertheless, there are instances where exceptions occur, as seen in Ch2 and Ch3. Even though Ch3 has the same molecular weight as Ch1, it has a higher melting point. The different colors of the compounds show differences in their electronic structure and chemical bonding, which could affect their usefulness for different things, like making dyes and chemical mixtures. While the molecular formula provides information on the compound's composition and the quantity of atoms for each element, it directly influences the molecular weight and melting point. For instance, the inclusion of chlorine in Ch1 and Ch4 elevates the molecular mass and influences the hue.

Table 2 displays the compounds prepared by the Claisen–Schmidt method using NaOH as a catalyst and benzaldehyde and ketone substituents.

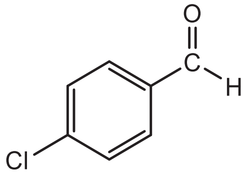
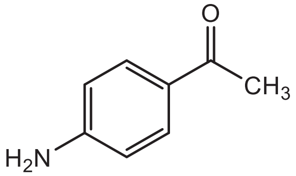
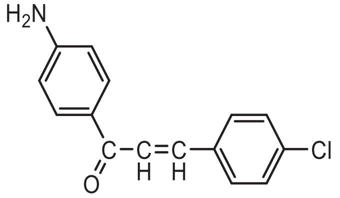
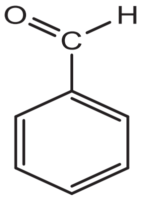
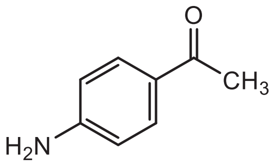
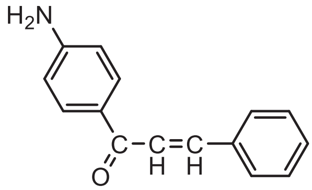
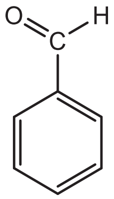
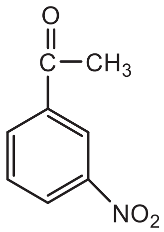
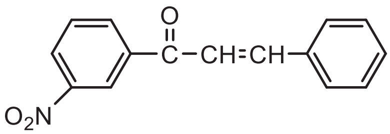
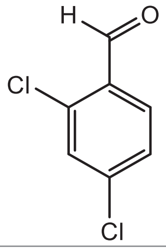
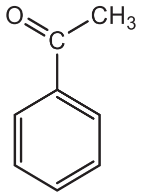
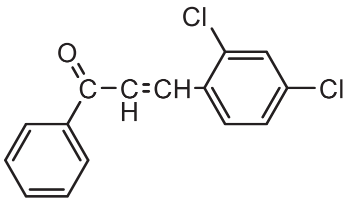
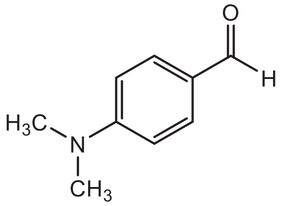
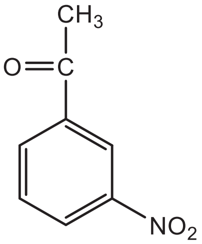
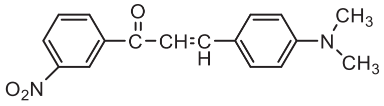
Study of UV-Vis photometry

The organic compound (Ch1) absorbs light in the UV wavelength range of 290-400 nm,[22] which corresponds to the conjugated α, β-unsaturated carbonyl (C=O) chromophore. This absorption is highlighted in Fig. 4, with a peak at 330 nm (λmax).Compound (Ch2) absorbs UV light in the range of 280-420 nm, with its maximum absorption occurring at 380 nm (λmax).Compound (Ch3) shows absorption across the UV wavelength range of 300-400 nm, with its peak absorption at 340 nm (λmax). Compound (Ch4) absorbs UV radiation within the wavelength range of 280-400 nm, reaching its highest absorption peak at 390 nm as seen in Fig. 5. Compound (Ch5) displays absorption in the UV wavelength range of 300-400 nm, with its strongest absorption observed at 390 nm.[23] These absorption characteristics are illustrated in Fig. 6.

FT-IR spectra for compounds

The compounds synthesized were analyzed utilizing FTIR technology and the findings are shown in Table 3. The band associated to the carbonyl groups (C=O) of the chalcone derivative is seen at a wavenumber spectrum of 1674-1647 cm^{-1}. The detection of two aromatic peaks at (1489-1586) cm^{-1} was also demonstrated. Two bands of absorption appear at the wavenumbers of 3050-2959 cm^{-1}, corresponding to the stretching vibrations of the C-H bonds

Table 2. Claisen-Schmidt condensation reaction catalyzed by NaOH 10%.

No of compound	Aldehydes	Ketones	Chalcones	Yield (%)
Ch1				65%
Ch2				91%
Ch3				92%
Ch4				68%
Ch5				60%

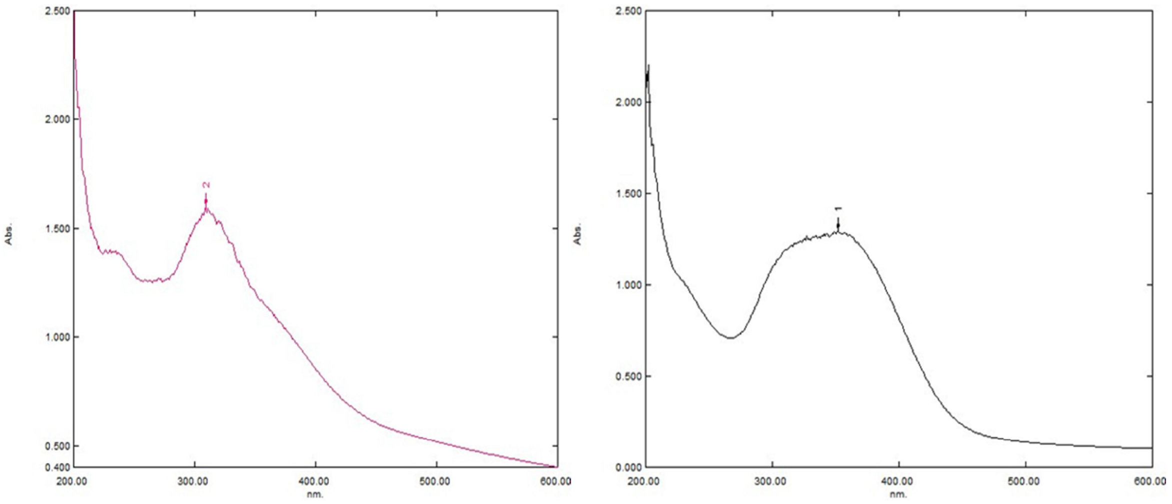
in the aromatic and aliphatic groups, respectively. The spectra of the compounds revealed to the band at (1654) cm^{-1}, which coincides with the carbonyl group's (C=O) stretching vibration. The scopes seen at 3074 cm^{-1}, 3057 cm^{-1}, 2089 cm^{-1}, and correspond to the vibrations caused by stretching of (C-H) bonds in aliphatic,[24] alkene, and aromatic compounds, respectively. At 1665-1660 cm^{-1}, the bands correspond to stretching vibrations in the C=C bond[25,26] As shown in Figs. 7 to 11.

^1H&^{13}C-NMR results

The ^1H-NMRand ^{13}C-NMR data for all compounds (Ch1, Ch2, Ch3, Ch4, Ch5) was obtained using DMSO as a solvent in the process. The results indicated the presence of (S,1H, at position C4) with a chemical shift range of (δ 8.66-8.25) ppm, α-H with a range of 6.17-6.45 ppm, β-H with a range of 6.37-6.99 ppm, and aromatic protons with a range of 7.22-8.17 ppm. (-OCH3) at 3.97 ppm,[27] as in Table 4. and Figs. 12 to 15

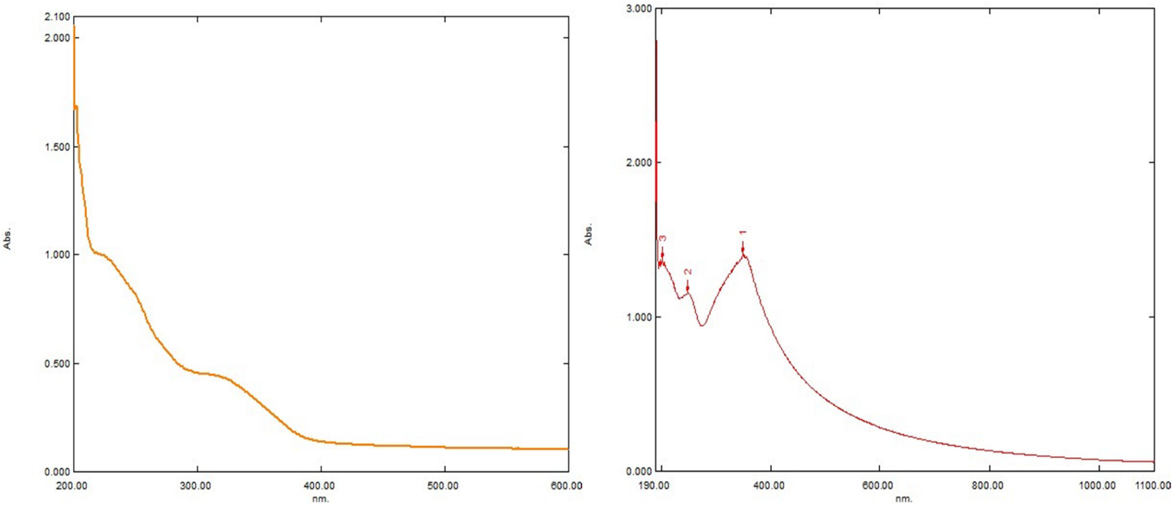
Theoretical study

Quantum descriptors such as electronegativity (χ), energy gap (ΔEgap), hardness (η), softness (σ), electron of highest occupied molecular orbital (EHOMO), and energy of lowest unoccupied molecular orbital (ELUMO) were estimated. The tendency of an atom



(Ch1) **(Ch2)**

Fig. 4. The UV-vis spectra of compound (Ch1), and (Ch2).



(Ch3) **(ch4)**

Fig. 5. The UV-vis spectra of compound (Ch3) and (Ch4).

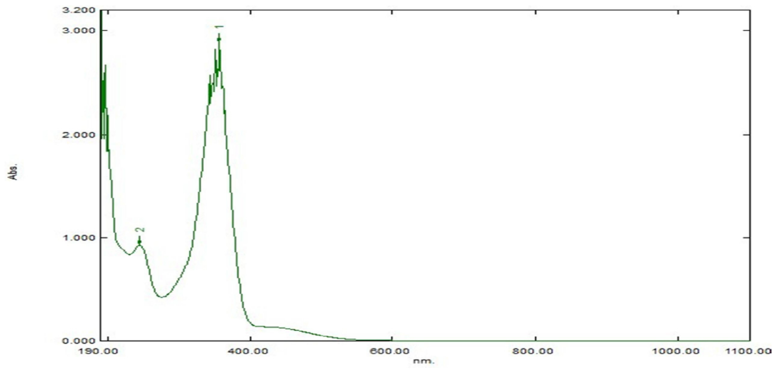


Fig. 6. The UV-vis spectra of compound (Ch5).

Table 3. Exhibits the compound's fourier transform infrared (FT-IR) spectrum.

Comp. No.	C-H aromatic	C=C aromatic	C=C olefinic	C=O	Others	
Ch1	3338 cm^{-1}	1562 cm^{-1}	1629 cm^{-1}	1653 cm^{-1}	C-Cl_2	823 cm^{-1}
					C-NH_2	3217 cm^{-1}
Ch2	3051 cm^{-1}	1593 cm^{-1}	1627 cm^{-1}	1653 cm^{-1}	NH_2	3338 cm^{-1}
Ch3	3086 cm^{-1}	1573 cm^{-1}	1610 cm^{-1}	1660 cm^{-1} 1687 cm^{-1}	NO_2	1525 cm^{-1}
Ch4	3059 cm^{-1}	1579 cm^{-1}	1604 cm^{-1}	1670 cm^{-1}	C-Cl_2	821 cm^{-1}
Ch5	2895 cm^{-1}	1585 cm^{-1}	1647 cm^{-1}	1519 cm^{-1} 1564 cm^{-1}	C-NO_2	1336 cm^{-1} 1363cm^{-1}
					C-N	2812cm^{-1}

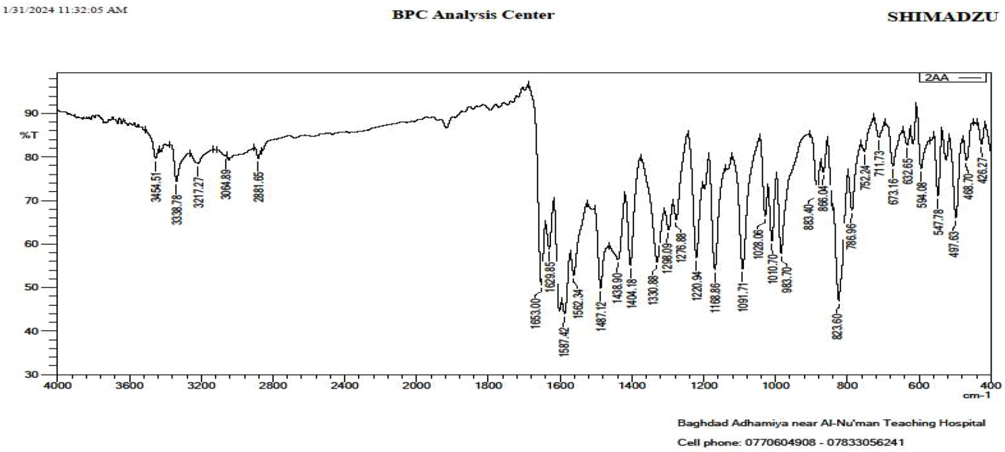


Fig. 7. The fourier transform infrared spectrum of compound (Ch1).

or group to draw electrons to itself while combining with another atom is known as electronegativity (χ). The following Eqs. (1) to (4) can be used to express it, according to DFT.[28] Table 5 shows that the electronegativity of Chalcones derivative are in the following order: Ch5 > Ch4 > Ch1 > Ch2 > Ch3.

$$\chi = I + A2 \quad (1)$$

$$I = -E_{HOMO} \quad (2)$$

$$A = -E_{LOMO} \quad (3)$$

$$\eta = I - A2 \quad (4)$$

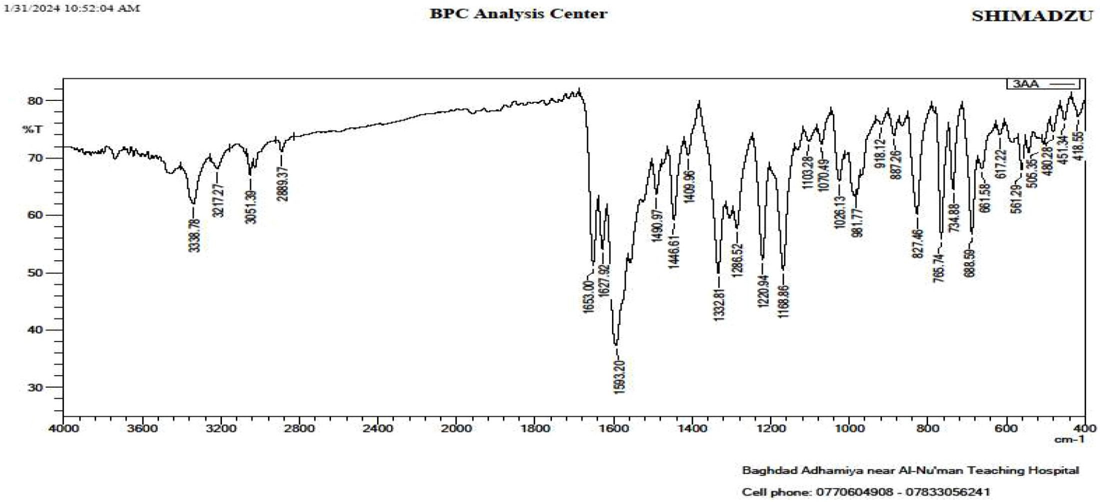


Fig. 8. The fourier transform infrared spectrum of compound (Ch2).

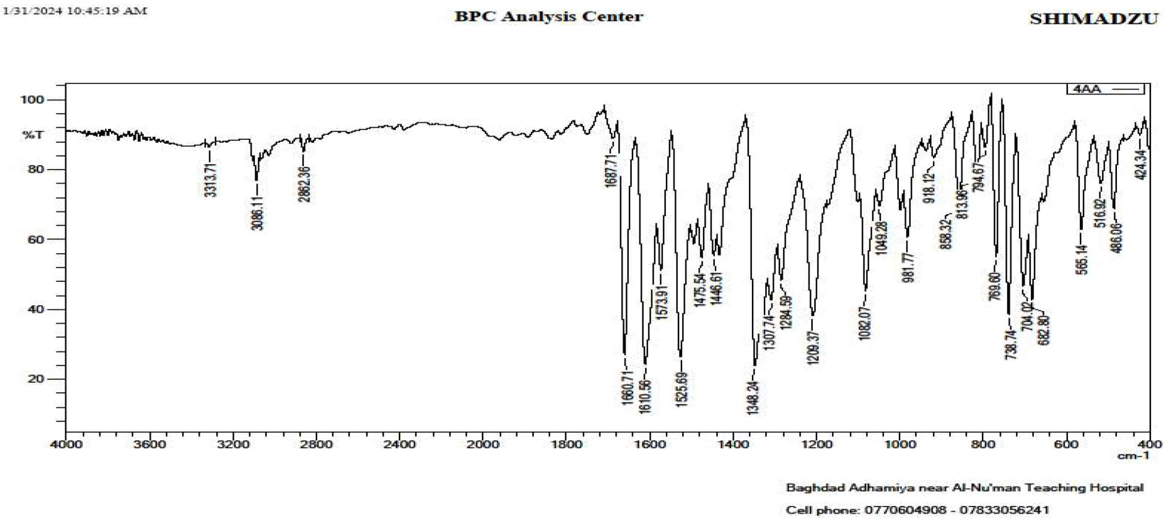


Fig. 9. The fourier transform infrared spectrum of compound (Ch3).

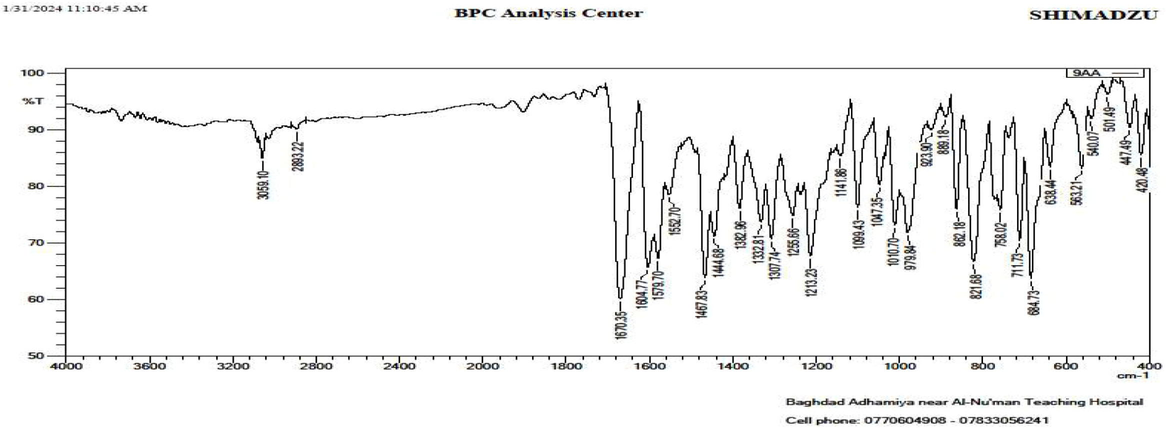


Fig. 10. The fourier transform infrared spectrum of compound (Ch4).

Ionization potential (I), electron affinity (A), electronegativity (χ), hardness (η),

Low energy species tend to receive electron donations from high E_{HOMO} levels. Elevations in E_{HOMO} values impact an inhibitor's capacity to inhibit. This is because the transport process has an impact on the metallic surface.[29] The adsorption of the inhibitor to the metal surface is directly proportional to the value of EHOMO. According to Table 5computed data, the order of E_{HOMO} is Ch4 > Ch5 > Ch1 > Ch2 > Ch3. Since it will take less energy to lose an electron in the last occupied orbital, a lower value of ΔE_{gap} will generally result in an increase in inhibition potency.

Koopman's theorem states that a molecule's ionisation energy and electron affinity are roughly correlated with the negative values of E_{HOMO} and E_{LUMO}.[30] Eqs. (1) and (2) can be used to calculate the ionization energy and electron affinity. An atom's or a group's tendency to draw electrons towards it is known as electronegativity (χ). There will be a partial transition of the electron from lower to higher electronegativity. Electrons can be readily transferred to the metal surface by a good inhibitor. A good inhibitor will therefore have a low electronegativity value.

The ability of the electron cloud of molecules to resist polarisation or deformation is known as chemical hardness.[31] Metals are regarded as hard acids according to Pearson's hard-soft-acid-base (HSAB) principle. On the other hand, corrosion inhibitors function as soft bases. The most efficacious inhibitor is expected to be a delicate compound with a lower hardness value.[32] The hardness values of Chalcone's derivative are shown in Table 5 in the following order:

Ch1 > Ch2 > Ch4 > Ch3 > Ch5 chemical system can be set up based on the Principle of Maximum Hardness (PMH) to obtain the highest possible hardness value. In other words, molecules that have a high

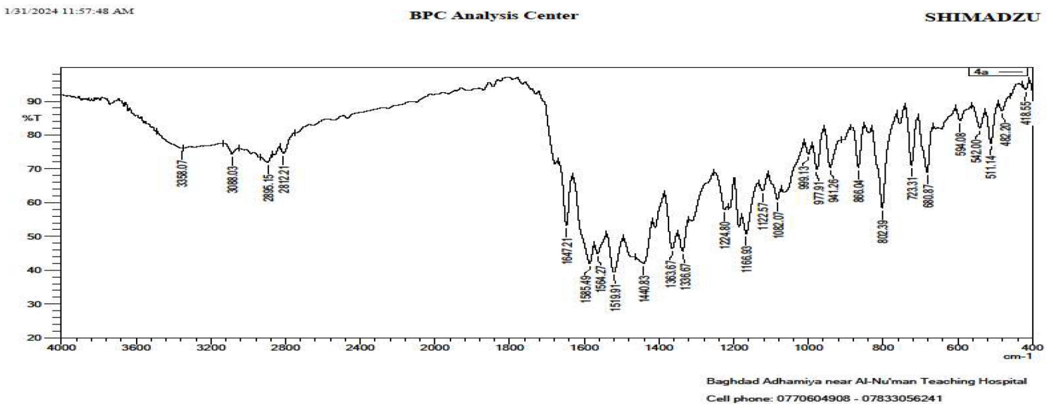
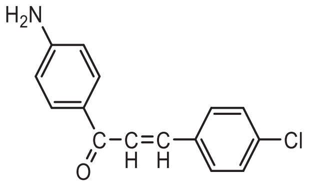
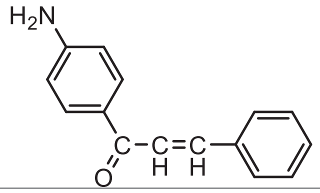
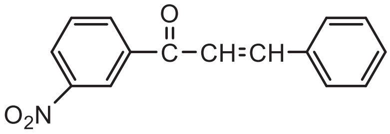
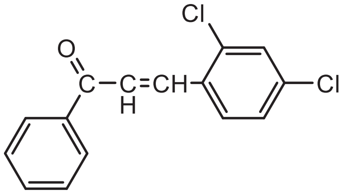
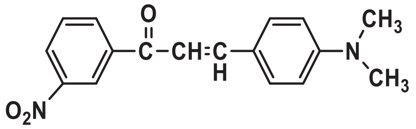


Fig. 11. The fourier transform infrared spectrum of compound (Ch5).

Table 4. Chemical shift data of ^{1}H-NMR and ^{13} C-NMR spectra of some chalcone derivatives.

Comp no	Structure	^{1}H NMR and ^{13}C NMR Spectral data (δ ,ppm)
Ch1		^{1}H NMR (300 MHz, DMSO) δ 8.66 (s, 1H), 8.25 (s, 1H), 8.22 (s, 1H), 8.04 (s, 1H), 7.99 (s, 2H), 7.96 (s, 3H), 7.93 (d, J = 3.5 Hz, 3H), 7.88 (s, 2H), 7.85 (s, 1H), 7.76 (s, 1H), 7.62 (s, 1H), 7.60 (s, 1H), 7.57 (s, 1H), 7.52 (s, 1H), 7.49 (d, J = 3.9 Hz, 3H), 7.46 (s, 1H), 7.40 (s, 1H), 7.37 (s, 1H), 6.65 (s, 2H), 6.62 (s, 1H), 6.21 (s, 2H), 3.41 (s, 2H). ^{13}C NMR (75 MHz, DMSO) δ 185.71, 178.64, 154.04, 139.97, 134.43, 134.19, 131.27, 130.65, 130.24, 128.89, 125.23, 123.22, 112.77, 96.67, 83.83, 40.36, 40.08, 39.80, 39.52, 39.24, 38.96, 38.68.
Ch2		^{1}H NMR (300 MHz, DMSO) δ 8.68 (s, 1H), 8.27 (s, 2H), 8.06 (s, 1H), 8.01 – 7.72 (m, 9H), 7.61 (d, J = 23.1 Hz, 4H), 7.49 – 7.35 (m, 7H), 6.74 – 6.44 (m, 2H), 6.15 (s, 1H). ^{13}C NMR (75 MHz, DMSO) δ 188.49, 163.03, 156.19, 144.24, 141.86, 136.14, 135.28 (d, J = 11.4 Hz), 132.49, 131.62, 130.56, 129.23 (d, J = 40.3 Hz), 122.85, 122.45, 121.74, 113.18.
Ch3		^{1}H NMR (300 MHz, DMSO) δ (ppm) (9.81 – 9.77 (m, 1H), 9.58 (d, J = 7.7 Hz, 2H), 9.45 (d, J = 8.2 Hz, 1H), 9.03 (s, 1H), 8.98 (s, 1H), 8.90 (s, 3H), 8.87 (s, 1H), 8.83 (t, J = 4.0 Hz, 3H), 8.77 (s, 1H), 8.45 (s, 4H). ^{13}C NMR (75 MHz, DMSO) δ 187.96, 148.64, 146.01, 139.14, 135.03 (d, J = 24.2 Hz), 131.49, 131.05, 129.54 (d, J = 22.2 Hz), 127.81, 123.32, 121.84, 40.78, 40.50, 40.22, 39.94, 39.67, 39.39, 39.11.
Ch4		^{1}H NMR (300 MHz, DMSO) δ(ppm) 8.16 (dd, J = 16.1, 8.2 Hz, 1H), 7.94 (d, J = 4.9 Hz, 1H), 7.65 – 7.40 (m, 2H). ^{13}C NMR (75 MHz, DMSO) δ 189.16, 137.63 (d, J = 8.8 Hz), 136.06, 135.62, 133.78 (d, J = 11.1 Hz), 131.73, 130.02 (d, J = 24.3 Hz), 129.17 (d, J = 8.5 Hz), 128.35 (d, J = 8.6 Hz), 125.50, 43.42, 32.66.
Ch5		^{1}H NMR (300 MHz, DMSO) δ (ppm) 8.83 – 8.29 (m, 1H), 7.75 – 7.68 (m, 1H), 6.74 (t, J = 9.1 Hz, 1H). ^{13}C NMR (75 MHz, DMSO) δ 147.97 (d, J = 95.5 Hz), 141.70 – 128.17 (m), 131.91 (d, J = 18.4 Hz), 127.57 (d, J = 57.6 Hz), 122.57 (d, J = 59.7 Hz), 111.82 (d, J = 47.5 Hz), 40.50, 40.22, 40.00 – 39.38 (m), 39.10.

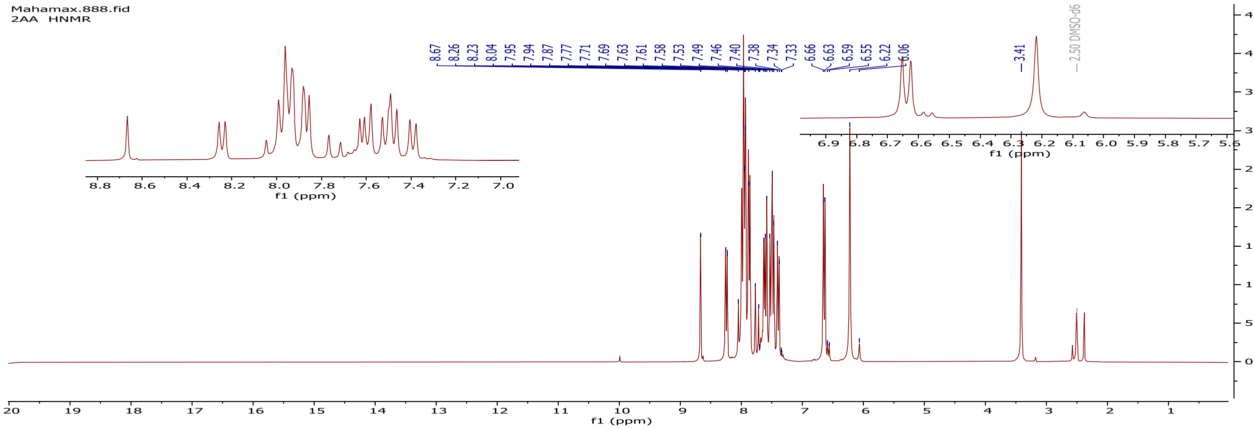


Fig. 12. H-NMR spectrum of compound (Ch1).

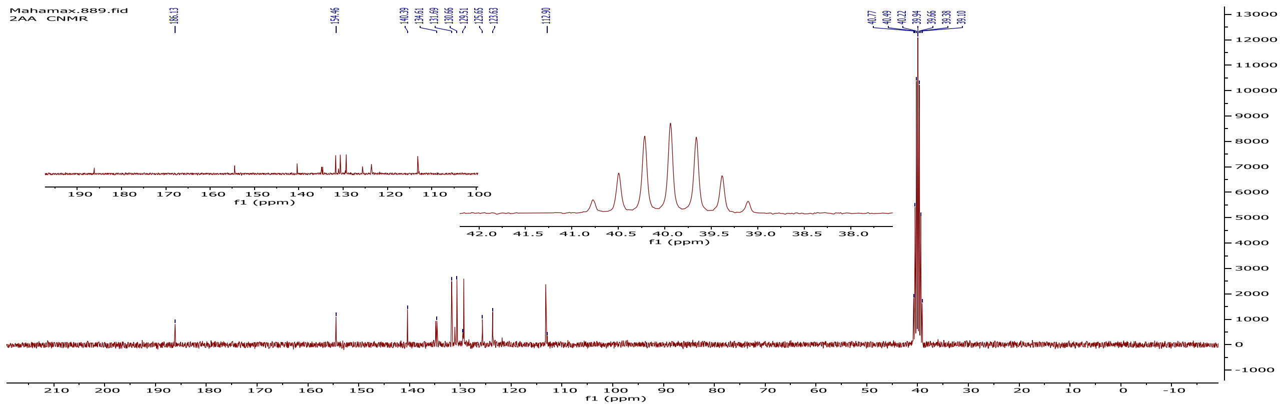


Fig. 13. C-NMR spectrum of compound (Ch1).

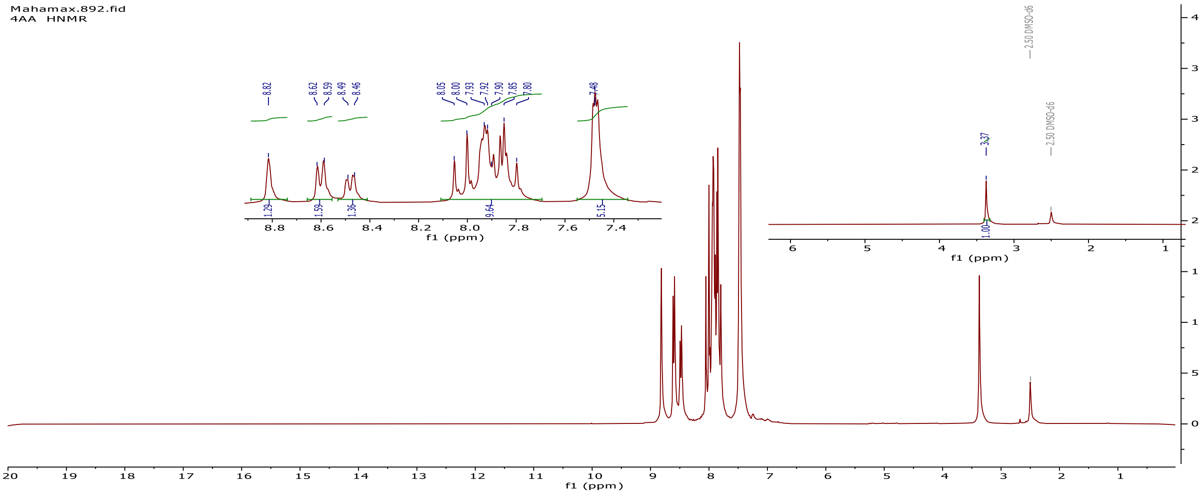


Fig. 14. C-NMR spectrum of compound (Ch3).

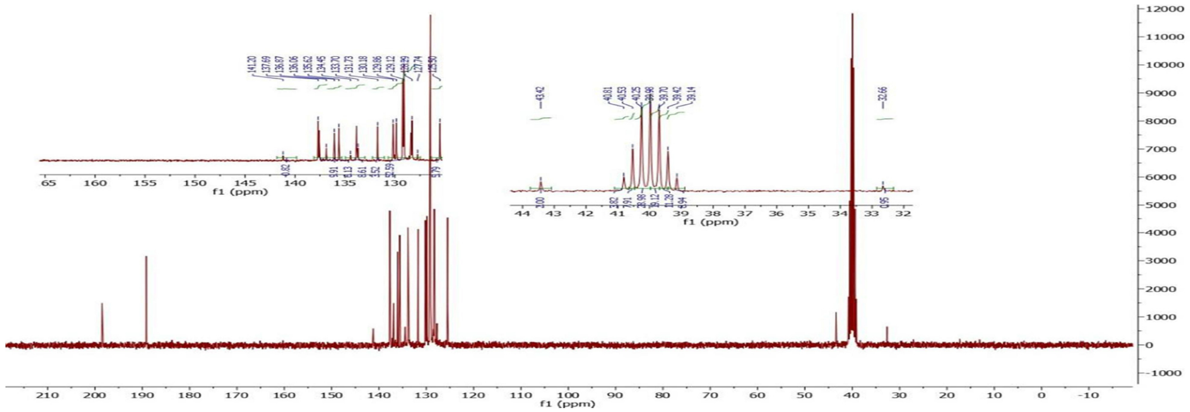


Fig. 15. C-NMR spectrum of compound (Ch4).

Table 5. Theoretical calculation of EHOMO, ELUMO, ΔE (eV), ionization potential (I), electron affinity (A), global hardness η, electronegativity χ for chalcone derivatives.

No of Compound	E_{HOMO}	E_{LUMO}	ΔE (eV)	Ionization potential (I)	Electron affinity (A)	Global hardness η	Electronegativity χ
Ch5	-9.559 ev	-6.009 ev	3.55	9.559 ev	6.009 ev	1.8	3.01
Ch2	-10.937 ev	-6.107 ev	4.83	10.937 ev	6.107 ev	2.4	8.5
Ch3	-10.963 ev	-6.964 ev	3.99	10.963 ev	6.964 ev	1.99	8.96
Ch4	-6.072 ev	-1.506 ev	4.6	6.072 ev	1.506 ev	2.3	3.8
Ch1	-10.704 ev	-5.575 ev	5.13	10.704 ev	5.575 ev	2.7	8.12

hardness value have a low effectivity of corrosion inhibitor efficiency.[33]

Conclusion

We have synthesized a number of chalcone derivatives by Claisen-Schmidt in 10% NaOH solution in the presence of various benzaldehyde and acetophenone substituents, such as Cl_2, $N(CH_3)_{2,}(Cl)$, NH_2 and NO_2 and characterized them using FT-IR, NMR, UV-vis spectroscopy. We studied them theoretically using Gaussian, a general-purpose computational chemistry software package. Chalcone derivatives have the potential to act as electron donors as anti-corrosion agents, and the derivative 3-(4-dimethylamino)phenyl)-1-(3-nitrophenyl)-prop-2-en-1, referred to as ch5 in the paper, was found to be the most effective corrosion inhibitor according to the equations used.

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Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the figures and tables in the manuscript are ours. Besides, figures and images, which are not ours have been given the permission for re-publication attached with the manuscript.
- No human studies are presented in manuscript.
- No animal studies are presented in manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Baghdad.

Authors' contributions statement

A.J.H conducted the practical side of the research, analyzed the results and wrote the manuscript. H.H. J & K.A.A conceived idea, supervised the research, contributed to the analysis of the results, and revised and proofread the manuscript.

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تحضير وتشخيص مشتقات الجالكون ودراستها نظريا لتثبيط التاكل

ايسر جمعة حمد[1]، حمدية حاتم جواد[1]، كاظم عبد الواحد عادم[2]

[1] *قسم الكيمياء، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق.*

[2] *قسم الفيزياء، كلية العلوم، جامعة بغداد، بغداد، العراق.*

المستخلص

تم التركيز في هذا البحث على تحضير عدد من مشتقات الجالكون بطريقة تفاعل كلايزن- شميت من خلال تفاعل بعض مشتقات البنزالديهايد مع مشتقات الأسيتوفينون في وجود وسط قاعدي يتمثل بـ (NaOH) بتركيز 10%. تم أيضًا إذابة مشتقات البنزالديهيد ومشتقات الأسيتوفينون في الإيثانول بتركيز 98٪. قبل البدء بالتحضير تم تحضير عدد من مشتقات الجالكون والتي يشار إليها بـ [Ch1، Ch2، Ch3، Ch4، Ch5]. المعوضات التي تم استخدامها في التحضير هي 4-كلوروبنزيتوفينون، 4-أمينو أسيتوفينون، بنزالدهيد، 3-نيتروسيتوفينون، 4-نيتروبنزايدهيد. أسيتوفينون، 2-4-ثنائي كلوروبنزالديهايد، و4-(ثنائي ميثيل أمينو)بنزالديهيد. تم تشخيص المركبات الناتجة طيفياً باستخدام (FT-IR ,1H NMR ,13C NMR وUV-Vis).. وبعد ذلك تم إجراء الدراسات النظرية للمركبات المحضرة كمثبطات للتآكل. وقد تمت دراستهم نظريًا باستخدام حزمة برامج الكيمياء الحاسوبية Gaussian. تتميز مشتقات الجالكونات مانحة للإلكترون كعوامل مضادة للتآكل. وقد وجد أن المشتق Ch5 أكثر فعالية كمثبط للتآكل نظريا.

الكلمات المفتاحية: تحضير، تشخيص، مشتقات الجالكون، الدراسة النظرية، مثبطات تاكل.