

# Analysis And Evaluation Of Novel Derivatives Of Chalcones For Their Antioxidant Capabilities

Tonukunuru Gopikishan

Ph.D Scholar, Department of Chemistry, Glocal University, India.

Email: [gkishan.org@gmail.com](mailto:gkishan.org@gmail.com)

Dr Harbeer Singh

Associate Professor, Department of Chemistry, Glocal University, India.

Email: [amansharma3568@gmail.com](mailto:amansharma3568@gmail.com)

**Abstract**-Chalcone, an important compound in the process of producing flavonoids, has been proven to have many biological and pharmacological characteristics, such as anti-inflammatory, antioxidant, and anti-cancer activities. In this study, the chalcones were chemically combined with either palmitic or stearic acid to produce a distinct set of chalcones fatty acid esters 5b-e and 6b-e. Additionally, two other classes of compounds have been synthesized through electrophilic and Michael addition reactions. These compounds include 2-amino-6-(substituted-phenyl)-4-substitutedphenyl-nicotinonitrile derivatives 9a, c, and e, as well as 2,3-disubstituted chalcones 7b-d and 8b(b')-d. The reactions were carried out using the corresponding chalcones. The structures of all compounds are confirmed through the utilization of diverse spectroscopic techniques, including mass spectra, <sup>1</sup>H and <sup>13</sup>C NMR, and infrared spectroscopy. 1,1-biphenyl-2-picrylhydrazyl was employed as a reagent to scavenge free radicals and assess the antioxidant capabilities of all synthesized compounds. The findings indicated that compound 5e exhibited higher antioxidant activity (68.58% at C = 2 µg/ml) compared to ascorbic acid, a commonly employed antioxidant. This discovery was unexpected. Conclusion: Chalcone fatty acid esters exhibited favorable activity, with certain members demonstrating superior antioxidant activity compared to ascorbic acid. In addition, the impact and contribution of different functional groups on the antioxidant activity of the produced chalcone derivatives are investigated and explained based on their electrical and structural influence.

**Keywords:** DPPH, Antioxidant activity, Fatty acid, and chalcones.

## I. INTRODUCTION

Studies have shown that both naturally occurring chalcones and their synthesized analogs possess diverse and fascinating biological and pharmacological properties. These properties include the ability to combat cancer, act as an antioxidant, decrease inflammation, fight against microbes, and enhance the immune system [1-4]. They appear to be offering cancer chemotherapy prophylactic medications that can be ingested with regular food consumption. Chalcones are commonly synthesized by combining aromatic aldehydes and aryl ketones with suitable condensing agents. The influence of the substitution patterns on the two aryl rings of chalcone molecules, known as the aryl moieties,

significantly affects the antioxidant capacities of chalcones. This is particularly important to the current research. It has been shown that the hydroxyl substituent can be easily transformed into phenol radicals by the hydrogen atom transfer mechanism. In this respect, it has been established that the hydroxyl group is one of the crucial components that greatly enhances the antioxidant activity of chalcone [5].

In light of these findings, Torres de Pinedo et al. [6-8] investigated the antioxidant properties of various phenolic compounds and found that galloyl alcohol (3,4,5-trihydroxybenzylic alcohol) and dihydrocaffeoyl alcohol (3-(3,4-dihydroxyphenyl)-1-propanol) exhibit greater antioxidant activity than hydroxyl tyrosol. These compounds are more effective at neutralizing free radicals and protecting the oil matrix from becoming rancid. To effectively combat pathogenic microorganisms, it is crucial to explore novel frameworks for developing and producing new antioxidant compounds, given their significant demand. Considering this, we offer straightforward procedures and techniques that enable the synthesis of novel chalcone fatty acid esters by directly attaching a fatty acid component to a phenolic site. In addition, we conducted experiments to determine the ability of chalcone fatty acid esters, which vary in the position of acylation in the phenol ring, as well as the length and composition of the fatty acid attached to the phenol ring, to scavenge radicals. The purpose of this study was to identify the specific structural characteristics that contribute to a compound's effectiveness as a lipophilic antioxidant. Furthermore, various addition and condensation processes of the necessary chalcones have been examined to get further insights into the influence of the double bond and the carbonyl group on antioxidant activity. The antioxidant test utilized in this study is important as it evaluates the synthesized compounds' capacity to eliminate 1,1-diphenyl-2-picrylhydrazyl (DPPH) radicals. The maximum absorption wavelength of DPPH, a stable radical, is 516 nm [9-11].

## II EXPERIMENTAL SECTION

In general SD Fine Chemicals and Merck supplied all the necessary chemicals for synthesizing the relevant compounds. The IA9000 series digital capillary melting point apparatus from Electrothermal was used to ascertain melting points, without any modifications. IR spectra were obtained using KBr discs and a 1000-Perkin Elmer FT-IR

spectrophotometer. The spectroscopic data were acquired using TMS as an internal standard to obtain  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra. The measurements were performed on a JEOL ECP-600 NMR instrument in  $\text{CDCl}_3$  (or  $\text{DMSO-d}_6$ ) solvent. The units of chemical changes are expressed as  $\delta$  parts per million (ppm). Mass spectra were acquired using a VL detector with an electron energy of 4000 V and a direct inlet system with an electron energy of 70 eV.

The standard procedure for synthesizing the derivatives 3a–e of 1,3-diphenylpropenone is as outlined below:

Following agitation at a temperature of  $25^\circ\text{C}$  for a duration of two to three hours, a combination of NaOH (22 g, 0.55 mol), acetophenone derivatives 1a–c (0.43 mol), and benzaldehyde derivatives 2a–d (0.43 mol) was subsequently refrigerated overnight. The yellow crystals were acquired by separating the solid that formed, purifying it with ethanol and water, drying it, and then recrystallizing it using ethanol.

The compounds (E)-3-(3-(substituted phenyl) acryloyl) phenyl or (E)-3-(3-(substituted phenyl)-3-oxoprop-1-en-1-yl)phenyl palmitate stearate (5b–e) and (E)-3-(3-(substituted phenyl) acryloyl)phenyl or (E)-3-(3-(substituted phenyl)-3-oxoprop-1-en-1-yl)phenyl stearate (6b–e) were synthesized.

At a temperature of  $25^\circ\text{C}$  in a controlled atmosphere of argon, a quantity of 2.68 millimoles of thionyl chloride (equivalent to 0.12 millilitres) was introduced into a mixture of fatty acid 4a–b (0.08 millimoles) suspended in dry  $\text{CH}_2\text{Cl}_2$ . Subsequently, the mixture was stirred vigorously for a duration of one hour. Following the addition of one equivalent of each chalcone and DMAP in pyridine, the mixture was stirred for a duration of one minute. The organic phase was extracted using water and diethyl ether. The extracted phase was subsequently dried with sodium carbonate ( $\text{Na}_2\text{SO}_4$ ), concentrated until it was completely dry, and purified using column chromatography (hexane–ethyl acetate, 9:1) to obtain 5b–e and 6b–e. The compound (E)-3-(3-(3,5-dimethoxyphenyl) acryloyl)phenyl palmitate (5b) was obtained as a yellow powder with a yield of 62% and a melting point (m.p.). The compound has a boiling point of  $116^\circ\text{C}$  and a molecular ion peak at  $m/z$  522  $[\text{M}^+]$ . Its molecular formula is  $\text{C}_{33}\text{H}_{46}\text{O}_5$ . In the infrared spectrum, there are absorption bands at  $1702\text{ cm}^{-1}$  corresponding to the  $\text{C}=\text{O}$  stretch in the ester group and at  $1654\text{ cm}^{-1}$  corresponding to the  $\text{C}=\text{O}$  stretch in the ketone group. The  $^1\text{H}$  NMR spectrum (recorded in  $\text{CDCl}_3$ ) shows peaks at 0.87 ppm (triplet, 3H,  $-\text{CH}_3$ ), 1.24 ppm (multiplet, 24H,  $-\text{CH}_2-$ ), 1.62 ppm (quartet, 2H,  $-\text{OCO}-\text{CH}_2-\text{CH}_2-$ ), 2.34 ppm (triplet, 2H,  $-\text{OCO}-\text{CH}_2$ ), 3.83 ppm (singlet, 6H,  $\text{OCH}_3$ ), 6.52 ppm (triplet, 1H, H-4), 6.76 ppm (doublet, 2H, H-2 & H-6), 7.1 ppm (doublet of doublets, 1H, H-4'), 7.37 ppm (triplet, 1H, H-5'), 7.45 ppm (doublet, 1H,  $J = 15.70\text{ Hz}$ , H- $\alpha$ ), 7.55 ppm (singlet, 1H, H-2'), 7.58 ppm (doublet, 1H, H-6'), and 7.72 ppm (doublet, 1H,  $J = 15.70\text{ Hz}$ , H- $\beta$ ). The  $^{13}\text{C}$  NMR spectrum of the compound in  $\text{CDCl}_3$  shows the following chemical shifts: 13.2 ppm ( $-\text{CH}_3$ ), 21.7 ppm ( $-\text{CH}_2-\text{CH}_3$ ), 23.7 ppm ( $-\text{CH}_2-\text{CH}_2-\text{CH}_3$ ), 28.5 ppm ( $-\text{CH}_2-$ ), 30.9 ppm ( $-\text{CH}_2-\text{CH}_2-\text{COO}-$ ), 33.1 ppm ( $-\text{CH}_2-\text{COO}-$ ), 54.5 ppm ( $-\text{OCH}_3$ ), 102 ppm (C-4), 105.5 ppm (C-2 & 6), 114.2 ppm (C-

2)), 119.4 ppm (C-6)), 120.1 ppm (C-4)), 121.5 ppm (C- $\alpha$ ), 129 ppm (C-5)), 135.7 ppm (C-1), 138.5 ppm (C-1)), 144.4 ppm (C- $\beta$ ), 155.4 ppm (C-3)), 160.1 ppm (C-3 & 5), 179.2 ppm ( $-\text{COO}-$ ), 189.7 ppm ( $-\text{C}=\text{O}$ ).

Phenyl palmitate (5c) (E)-3-(3-(4-bromophenyl) acryloyl) is a yellow powder with a yield of 84% and a melting point. The compound has a boiling point of  $126^\circ\text{C}$  and a molecular ion peak at  $m/z$  540  $[\text{M}^+]$ . Its molecular formula is  $\text{C}_{31}\text{H}_{41}\text{BrO}_3$ . The infrared spectrum shows absorption peaks at  $1702\text{ cm}^{-1}$ , indicating the presence of an ester group, and at  $1654\text{ cm}^{-1}$ , indicating the presence of a ketone group. The  $^1\text{H}$  NMR spectrum in  $\text{CDCl}_3$  solvent shows peaks at 0.87 ppm (triplet, 3H,  $-\text{CH}_3$ ), 1.24 ppm (multiplet, 24H,  $-\text{CH}_2-$ ), 1.62 ppm (quartet, 2H,  $-\text{OCO}-\text{CH}_2-\text{CH}_2-$ ), 2.34 ppm (triplet, 2H,  $-\text{OCO}-\text{CH}_2$ ), 7.08 ppm (doublet, 1H, H-4'), 7.39 ppm (triplet, 1H, H-5'), 7.52 ppm (multiplet, 7H, H-2, 6, 3, 5,  $\alpha$ , 2', 6'), and 7.74 ppm (doublet, 1H,  $J = 15.60\text{ Hz}$ , H- $\beta$ ). 13.0 (methyl group), 21.6 (ethyl group), 23.6 (propyl group), 28.4 (methylene group), 30.6 (ethyl ester group), 33.1 (carboxylate group), 113.8 (carbon atom 2), 119.5 (carbon atom alpha), 119.8 (carbon atom 6), 121.2 (carbon atom 4), 123.9 (carbon atom 4), 128.6 (carbon atoms 2, 6, and 5), 131.1 (carbon atoms 3 and 5), 132.5, The chemical shifts are as follows: C-1 is at 138.3 ppm, C-1' is at 142.4 ppm, C- $\beta$  is at 155.4 ppm, C-3 is at 175.4 ppm,  $-\text{COO}-$  is at 189.3 ppm, and  $-\text{C}=\text{O}$  is at 189.3 ppm.

The compound (E)-3-(3-(4-bromophenyl)-3-oxoprop-1-en-1-yl)phenyl palmitate (5d) is a pale powder obtained with a 62% yield and has a melting point (m.p.). The compound has a melting point of  $132^\circ\text{C}$  and a molecular ion peak at  $m/z$  540  $[\text{M}^+]$ . Its molecular formula is  $\text{C}_{31}\text{H}_{41}\text{BrO}_3$ . In the infrared spectrum, there are absorption bands at  $1704\text{ cm}^{-1}$  corresponding to the  $\text{C}=\text{O}$  stretch in the ester group and at  $1652\text{ cm}^{-1}$  corresponding to the  $\text{C}=\text{O}$  stretch in the ketone group. The  $^1\text{H}$  NMR spectrum (recorded in  $\text{CDCl}_3$ ) shows peaks at 0.83 ppm (triplet, 3H,  $-\text{CH}_3$ ), 1.24 ppm (multiplet, 28H,  $-\text{CH}_2-$ ), 1.59 ppm (quartet, 2H,  $-\text{OCO}-\text{CH}_2-\text{CH}_2-$ ), 2.31 ppm (triplet, 2H,  $-\text{OCO}-\text{CH}_2$ ), 6.89 ppm (doublet, 1H, H-4), 7.11 ppm (singlet, 1H, H-2), 7.18 ppm (doublet, 1H, H-6), 7.26 ppm (triplet, 1H, H-5), 7.41 ppm (doublet, 1H,  $J = 15.70\text{ Hz}$ , H- $\alpha$ ), 7.61 ppm (doublet, 2H,  $J = 8.00\text{ Hz}$ , H-3 & 5)), 7.73 ppm (doublet, 1H,  $J = 15.70\text{ Hz}$ , H- $\beta$ ), and 7.85 ppm (doublet, 2H,  $J = 8.00\text{ Hz}$ , H-2' & 6'). The  $^{13}\text{C}$  NMR spectrum (recorded in  $\text{CDCl}_3$ ) shows the following chemical shifts: 12.9 ppm ( $-\text{CH}_3$ ), 21.5 ppm ( $-\text{CH}_2-\text{CH}_3$ ), 23.5 ppm ( $-\text{CH}_2-\text{CH}_2-\text{CH}_3$ ), 28.5 ppm ( $-\text{CH}_2-$ ), 30.7 ppm ( $-\text{CH}_2-\text{CH}_2-\text{COO}-$ ), 32.8 ppm ( $-\text{CH}_2-\text{COO}-$ ), 113.8 ppm (C-2), 116.9 ppm (C-4), 120.2 ppm (C-6), 120.6 ppm (C-alpha), 128.9 ppm (C-2 and C-6), 129.1 ppm (C-5), 130.8 ppm (C-3 and C-5), 134.9 ppm (C-4), 135.2 ppm (C-1), 136.8 ppm (C-1), 144.1 ppm (C-beta), 155 ppm (C-3), 178.4 ppm ( $-\text{COO}-$ ), and 188.4 ppm ( $-\text{C}=\text{O}$ ).

The substance is orange powder with a yield of 40% and a melting point. The compound is (E)-3-(3-(4-nitrophenyl)-3-oxoprop-1-en-1-yl)phenyl palmitate (5e). The compound has a melting point of  $182^\circ\text{C}$  and a molecular ion peak at  $m/z$  507  $[\text{M}^+]$ . Its molecular formula is  $\text{C}_{31}\text{H}_{41}\text{NO}_5$ . In the infrared spectrum, there are absorption bands at  $1701\text{ cm}^{-1}$

corresponding to the C=O stretch in the ester group and at 1653 cm<sup>-1</sup> corresponding to the C=O stretch in the ketone group. The <sup>1</sup>H NMR spectrum (recorded in CDCl<sub>3</sub>) shows peaks at 0.85 ppm (triplet, 3H, -CH<sub>3</sub>), 1.22 ppm (multiplet, 24H, -CH<sub>2</sub>-), 1.46 ppm (quartet, 2H, -OCO-CH<sub>2</sub>-CH<sub>2</sub>-), 2.17 ppm (triplet, 2H, -OCO-CH<sub>2</sub>), 6.90 ppm (doublet, 1H, H-4), 7.26 ppm (singlet, 1H, H-2), 7.27 ppm (doublet, 1H, H-6), 7.33 ppm (triplet, 1H, H-5), 7.70 ppm (doublet, 1H, J = 15.50 Hz, H-α), 7.86 ppm (doublet, 1H, J = 15.50 Hz, H-β), and 8.36 ppm (multiplet, 4H, H-2', 6', 3' & 5'). The <sup>13</sup>C NMR spectrum (recorded in CDCl<sub>3</sub>) shows the following chemical shifts: 13.3 ppm (for -CH<sub>3</sub>), 21.4 ppm (for -CH<sub>2</sub>-CH<sub>3</sub>), 23.8 ppm (for -CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>), 28.1 ppm (for -CH<sub>2</sub>-), 30.6 ppm (for -CH<sub>2</sub>-CH<sub>2</sub>-COO-), 33.0 ppm (for -CH<sub>2</sub>-COO-), 114.5 ppm (for C-2), 118.1 ppm (for C-4), 119.8 ppm (for C-6), 121.2 ppm (for C-α), 123.2 ppm (for C-2 & 6), 129.1 ppm (for C-5), 129.3 ppm (for C3 & 5), 135 ppm (for C-1), 141.6 ppm (for C-1~), 145.3 ppm (for C-β), 149.2 ppm (for C-3), 157.4 ppm (for C-4~), 173.8 ppm (for -COO-), and 187.9 ppm (for -C=O).

Phenyl stearate (E)-3-(3-(3,5-dimethoxyphenyl) acryloyl) (6b) is a yellow powder that was obtained with a 48% yield and has a melting point (m.p.). The compound has a melting point of 114°C and a molecular ion peak at m/z 540 [M<sup>+</sup>]. Its molecular formula is C<sub>35</sub>H<sub>50</sub>O<sub>5</sub>. In the infrared spectrum, there are absorption peaks at 1705 cm<sup>-1</sup> corresponding to the C=O bond in the ester group and at 1654 cm<sup>-1</sup> corresponding to the C=O bond in the ketone group. The <sup>1</sup>H NMR spectrum (recorded in CDCl<sub>3</sub>) shows peaks at 0.87 ppm (triplet, 3H, -CH<sub>3</sub>), 1.24 ppm (multiplet, 28H, -CH<sub>2</sub>-), 1.62 ppm (quartet, 2H, -OCO-CH<sub>2</sub>-CH<sub>2</sub>-), 2.34 ppm (triplet, 2H, -OCO-CH<sub>2</sub>), 3.83 ppm (singlet, 6H, OCH<sub>3</sub>), 6.52 ppm (triplet, 1H, H-4), 6.76 ppm (doublet, 2H, H-2 & H-6), 7.1 ppm (doublet of doublets, 1H, H-4), 7.38 ppm (triplet, 1H, H-5), 7.44 ppm (doublet, 1H, J = 15.30 Hz, H-α), 7.55 ppm (doublet, 1H, H-6), and 7.72 ppm (singlet, 1H, H-2).

J corresponds to a frequency of 15.3 Hz, namely in the H-β range. The <sup>13</sup>C NMR spectrum (recorded in CDCl<sub>3</sub>) shows the following chemical shifts: 13.1 ppm (-CH<sub>3</sub>), 21.7 ppm (-CH<sub>2</sub>-CH<sub>3</sub>), 23.7 ppm (-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>), 28.1 ppm (-CH<sub>2</sub>-), 30.9 ppm (-CH<sub>2</sub>-CH<sub>2</sub>-COO-), 33.1 ppm (-CH<sub>2</sub>-COO-), 54.5 ppm (-OCH<sub>3</sub>), 101.9 ppm (C-4), 105.4 ppm (C-2 & 6), 114.1 ppm (C-2), 119.2 ppm (C-6~), 120.1 ppm (C-4), 121.4 ppm (C-α), 128.9 ppm (C-5), 135.6 ppm (C-1), 138.7 ppm (C-1), 144.2 ppm (C-β), 155.1 ppm (C-3), 160 ppm (C-3 & 5), 179.5 ppm (-COO-), and 189.6 ppm (-C=O).

The compound (E)-3-(3-(4-bromophenyl) acryloyl) phenyl stearate (6c), which is a yellow powder, was obtained with a yield of 34%. It has a melting point (m.p.). At a temperature of 120°C, the compound has a molecular weight of 568 (m/z%) with the molecular formula C<sub>33</sub>H<sub>45</sub>BrO<sub>3</sub>. In the infrared spectrum, it shows absorption peaks at 1702 cm<sup>-1</sup> for the ester group and 1654 cm<sup>-1</sup> for the ketone group. In the <sup>1</sup>H nuclear magnetic resonance spectrum recorded in CDCl<sub>3</sub>, the compound exhibits signals at 0.87 ppm (triplet, 3H, -CH<sub>3</sub>), 1.24 ppm (multiplet, 28H, -CH<sub>2</sub>-), 1.62 ppm (quartet, 2H, -OCO-CH<sub>2</sub>-CH<sub>2</sub>-), 2.34 ppm (triplet, 2H, -OCO-CH<sub>2</sub>), 7.11 ppm (doublet, 1H, H-4), 7.37 ppm (triplet,

1H, H-5), 7.51 ppm (multiplet, 7H, H-2, 6, 3, 5, α, 2, 6), and 7.74 ppm (doublet, 1H, J = 15.70 Hz, H-β). The chemical shifts of the different carbon atoms in the compound are as follows: 13.0 ppm for the carbon atom with a methyl group (-CH<sub>3</sub>), 21.6 ppm for the carbon atom with an ethyl group (-CH<sub>2</sub>-CH<sub>3</sub>), 23.6 ppm for the carbon atom with a propyl group (-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>), 28.3 ppm for the carbon atom with a methylene group (-CH<sub>2</sub>-), 30.8 ppm for the carbon atom with an ethylene group (-CH<sub>2</sub>-CH<sub>2</sub>-COO-), 33.1 ppm for the carbon atom with a carboxyl group (-CH<sub>2</sub>-COO-), 114.1 ppm for the C-2 carbon atom, 119.5 ppm for the C-alpha carbon atom, 119.9 ppm for the C-6 carbon atom, 121.3 ppm for the C-4 carbon atom, 123.9 ppm for the C-4 carbon atom, 128.8 ppm for the C-2,6 and C-5 carbon atoms, 131.1 ppm for the C-3,5 carbon atoms, 132.6 ppm for the C-1 carbon atom, 138.3 ppm for the C-1 carbon atom, 142.8 ppm for the C-beta carbon atom, 155.2 ppm for the C-3 carbon atom, 175.4 ppm for the carboxyl group (-COO-), and 189.3 ppm for the carbonyl group (-C=O).

The compound (6d), which is a yellow powder, was synthesized with a yield of 66%. It has a melting point (m.p.). The compound's chemical name is (E)-3-(3-(4-bromophenyl)-3-oxoprop-1-en-1-yl)phenyl stearate. The compound has a melting point of 136°C and a molecular ion peak at m/z 568 [M<sup>+</sup>]. Its molecular formula is C<sub>33</sub>H<sub>45</sub>BrO<sub>3</sub>. In the infrared spectrum, there are absorption bands at 1704 cm<sup>-1</sup> corresponding to the C=O bond in the ester group and at 1652 cm<sup>-1</sup> corresponding to the C=O bond in the ketone group. The <sup>1</sup>H NMR spectrum (recorded in CDCl<sub>3</sub>) shows peaks at 0.87 ppm (triplet, 3H, -CH<sub>3</sub>), 1.24 ppm (multiplet, 28H, -CH<sub>2</sub>-), 1.62 ppm (quartet, 2H, -OCO-CH<sub>2</sub>-CH<sub>2</sub>-), 2.34 ppm (triplet, 2H, -OCO-CH<sub>2</sub>), 6.91 ppm (doublet, 1H, H-4), 7.14 ppm (singlet, 1H, H-2), 7.20 ppm (doublet, 1H, H-6), 7.29 ppm (triplet, 1H, H-5), 7.44 ppm (doublet, 1H, J = 15.70 Hz, H-α), 7.64 ppm (doublet, 2H, J = 8.40 Hz, H-3' & 5'), 7.76 ppm (doublet, 1H, J = 15.70 Hz, H-β), and 7.87 ppm (doublet, 2H, J = 8.40 Hz, H-2' & 6'). The <sup>13</sup>C NMR spectrum (recorded in CDCl<sub>3</sub>) shows the following chemical shifts: 12.9 ppm (-CH<sub>3</sub>), 21.5 ppm (-CH<sub>2</sub>-CH<sub>3</sub>), 23.5 ppm (-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>), 28.2 ppm (-CH<sub>2</sub>-), 30.8 ppm (-CH<sub>2</sub>-CH<sub>2</sub>-COO-), 32.8 ppm (-CH<sub>2</sub>-COO-), 113.8 ppm (C-2), 116.8 ppm (C-4), 120.1 ppm (C-6), 120.6 ppm (C-α), 128.9 ppm (C-2 & 6), 129.1 ppm (C-5), 130.8 ppm (C3 & 5), 135 ppm (C-4), 135.6 ppm (C-1), 137 ppm (C-1), 144.1 ppm (C-β), 155 ppm (C-3), 178.4 ppm (-COO-), 188.5 ppm (-C=O).

Phenyl stearate (6e) (E)-3-(3-(4-nitrophenyl)-3-oxoprop-1-en-1-yl) is a yellow powder with a yield of 54% and a melting point (m.p.). The compound has a melting point of 184°C and a molecular ion peak at m/z 535 [M<sup>+</sup>]. Its molecular formula is C<sub>33</sub>H<sub>45</sub>NO<sub>5</sub>. In the infrared spectrum, there are peaks at 1703 cm<sup>-1</sup> corresponding to the carbonyl group in the ester and 1653 cm<sup>-1</sup> corresponding to the carbonyl group in the ketone. The <sup>1</sup>H NMR spectrum in CDCl<sub>3</sub> solvent shows peaks at 0.87 (triplet, 3H, -CH<sub>3</sub>), 1.24 (multiplet, 24H, -CH<sub>2</sub>-), 1.62 (quartet, 2H, -OCO-CH<sub>2</sub>-CH<sub>2</sub>-), 2.34 (triplet, 2H, -OCO-CH<sub>2</sub>), 6.90 (doublet, 1H, H-4), 7.25 (singlet, 1H, H-2), 7.29 (doublet, 1H, H-6), 7.31 (triplet, 1H, H-5), 7.70 (doublet, 1H, J = 15.50 Hz, H-α), 7.84 (doublet, 1H, J = 15.50 Hz, H-β), and 8.36 (multiplet, 4H, H-2', 6', 3' & 5'). The <sup>13</sup>C

NMR spectrum in CDCl<sub>3</sub> shows peaks at 13.2 (–CH<sub>3</sub>), 21.5 (–CH<sub>2</sub>-CH<sub>3</sub>), 23.6 (–CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>), 28.2 (–CH<sub>2</sub>-), 30.7 (–CH<sub>2</sub>-CH<sub>2</sub>-COO-), and 32.8 (–CH<sub>2</sub>-COO-). Additionally, there is a peak at 114.7 corresponding to carbon atom C-2.

The following numbers represent different carbon atoms in a compound: 117.6 (C-4), 119.5 (C-6), 121 (C-α), 123.1 (C-2~& 6~), 128.8 (C-5), 129.2 (C3~& 5~), 135 (C-1), 141.7 (C-1~), 145.1 (C-β), 149.1 (C-3), 157.1 (C-4)}, 173.7 (–COO-), 187.7 (–C= O).

The synthesis of 2,3-Dibromo-1,3-diphenyl-propan-1-one derivatives (7b-d) involved swirling a mixture of chalcone derivatives 3b-d (1 mmol) and bromine (2 ml) in 25 ml of chloroform over a period of 1-4 hours. After the chilling process, ethanol was introduced, and the resulting solid was collected through filtration. The compound 7b-d, which consists of derivatives of 2,3-dibromo-1,3-diphenyl-propan-1-one, was produced as a white powder by recrystallization from ethanol.

The substance is a white powder with a yield of 80% and a melting point. The compound 2,3-Dibromo-3-(3,5-dimethoxy-phenyl)-1-(3-hydroxy-phenyl)-propan-1-one is referred. The compound has a melting point of 236°C and a molecular ion peak at m/z 442 [M<sup>+</sup>]. Its molecular formula is C<sub>17</sub>H<sub>16</sub>Br<sub>2</sub>O<sub>4</sub>. In the infrared spectrum, it shows absorption peaks at 3410 cm<sup>-1</sup> (indicating the presence of an OH group) and 1711 cm<sup>-1</sup> (indicating a ketone group). The <sup>1</sup>H NMR spectrum (recorded in CDCl<sub>3</sub>) shows the following signals: a singlet at 3.95 ppm (corresponding to 6 protons of a methoxy group), a singlet at 6.18 ppm (representing 1 proton at position 2), a singlet at 6.34 ppm (representing 1 proton at position 6), a doublet at 6.56 ppm (representing 1 proton at position 4), a doublet at 6.76 ppm (representing 1 proton at position 4'), a doublet at 6.85 ppm (with a coupling constant of 11.40 Hz, representing 1 proton at position β), a triplet at 6.86 ppm (representing 1 proton at position 5'), and a doublet at 7.02 ppm (with a coupling constant of 11.40 Hz, representing 1 proton at position α). Additionally, there are two singlets at 7.78 ppm, corresponding to 2 protons at positions 2' and 6'. The <sup>13</sup>CNMR spectrum of the compound in CDCl<sub>3</sub> shows the following chemical shifts: 45.78 ppm (C-β), 48.07 ppm (C-α), 56.71 ppm (–OCH<sub>3</sub>), 96.91 ppm (C-4), 105.32 ppm (C-2), 107.7 ppm (C-6), 112.31 ppm (C-2'), 122.08 ppm (C-4'), 131.94 ppm (C-6'), 135.9 ppm (C-5'), 136.8 ppm (C-1'), 138.32 ppm (C-1), 150.04 ppm (C-3'), 156.11 ppm (C-3), 156.38 ppm (C-5), and 188.94 ppm (C = O).

The compound is named Propan-1-one (7c)–2,3-Dibromo-3-(4-bromo-phenyl)-1-(3-hydroxy-phenyl). The product obtained has a yield of 82% and appears as a white powder with a melting point (m.p.). At a temperature of 300°C, the mass-to-charge ratio (m/z) is 460 [M<sup>+</sup>] for the compound C<sub>15</sub>H<sub>11</sub>Br<sub>3</sub>O<sub>2</sub>. Infrared spectroscopy (IR) shows absorption peaks at 3461 cm<sup>-1</sup> for the hydroxyl group (OH) and at 1709 cm<sup>-1</sup> for the carbonyl group (C = O) in the ketone. Proton nuclear magnetic resonance (<sup>1</sup>H NMR) in CDCl<sub>3</sub> solvent reveals the following chemical shifts: 5.56 (doublet, 1H, J = 10.80 Hz, H-β), 6.01 (doublet, 1H, J = 10.80 Hz, H-α), 7.41

(doublet, 2H, J = 8.40 Hz, H-2 & H-6), 7.53 (doublet, 2H, J = 8.40 Hz, H-3 & H-5), 7.60 (doublet, 1H, H-4'), 7.72 (triplet, 1H, H-5'), 7.78 (singlet, 1H, H-2'), 7.81 (doublet, 1H, H-6'). Carbon-13 nuclear magnetic resonance (<sup>13</sup>CNMR) in CDCl<sub>3</sub> shows the following chemical shifts: 46.95 (C-β), 51.96 (C-α), 114.42 (C-2'), 122.7 (C-4'), 129.92 (C-2 & C-6), 131.7 (C-6'), 131.72 (C-3 & C-5), 132.3 (C-4), 135.8 (C-5'), 137.9 (C-1), 138.01 (C-1'), 151.43 (C-3'), 189.38 (C = O).

The compound propan-1-one (7d) can be represented by the chemical formula 2,3-Dibromo-1-(4-bromo-phenyl)-3-(3-hydroxy-phenyl). Achieved a yield of 90%, resulting in a white powder with a melting point. At a temperature of 300°C, the mass-to-charge ratio (m/z) is 460 for the molecular ion [M<sup>+</sup>] of the compound C<sub>15</sub>H<sub>11</sub>Br<sub>3</sub>O<sub>2</sub>. In the infrared spectrum, the absorption peaks are observed at 3447 cm<sup>-1</sup> for the hydroxyl group (OH) and at 1683 cm<sup>-1</sup> for the carbonyl group (C = O) of the ketone. The proton nuclear magnetic resonance (<sup>1</sup>H NMR) spectrum in CDCl<sub>3</sub> solvent shows the following peaks: 6.21 (doublet, 1H, H-4), 6.61 (singlet, 1H, H-2), 6.64 (doublet, 1H, J = 11.40 Hz, H-β), 6.67 (doublet, 1H, J = 11.40 Hz, H-α), 7.66 (triplet, 1H, H-5), 7.70 (doublet, 2H, J = 8.50 Hz, H-3' & H-5'), 7.84 (doublet, 1H, H-6), and 7.93 (doublet, 2H, J = 8.50 Hz, H-2' & H-6'). The <sup>13</sup>CNMR spectrum of the compound in CDCl<sub>3</sub> shows the following chemical shifts: 111.1 ppm (C-4), 112.5 ppm (C-2), 114.95 ppm (C-6), 117.4 ppm (C-4'), 130.36 ppm (C-2' & C-6'), 132.45 ppm (C-3' & C-5'), 132.78 ppm (C-5), 135.5 ppm (C-1'), 137.01 ppm (C-1), 149.84 ppm (C-3), and 189.26 ppm (C = O).

The production of derivatives of 8b(b')-d, 2,3-Disubstituted-1,3-diphenyl-propan-1-one. A solution containing morpholine or piperidine (0.01 mol) and 2,3-dibromo-1,3-diphenyl-propan-1-one derivatives 7a-c (0.01 mol) in ethanol (10 ml) was heated in an oil bath for a duration of five hours. After cooling, the organic phase was separated by extracting it with 50 ml of water. This was followed by washing it three times with 10% hydrochloric acid (HCl) solution (each time using 50 ml), drying it with sodium carbonate (Na<sub>2</sub>SO<sub>4</sub>), and then evaporating it until it became dry. Following the isolation of the solid and its purification on silica gel using column chromatography with ethyl acetate/hexane (3:7) as the eluent, yellow powders of 2,3-disubstituted-1,3-diphenyl-propan-1-one derivatives 8a–d were produced.

The compound 3-(3,5-Dimethoxy-phenyl)-1-(3-hydroxy-phenyl)-2,3-di-piperidin-yl-propan The product has a yield of 50% and appears as a yellow-orange powder. Its melting point is not specified. The compound was heated to a temperature of 225°C. Its molecular weight percentage (m/z%) was found to be 452, with the molecular formula C<sub>27</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>. The infrared spectrum showed absorption peaks at 3427 cm<sup>-1</sup> (indicating the presence of an OH group) and 1634 cm<sup>-1</sup> (indicating the presence of a ketone group). The proton nuclear magnetic resonance (<sup>1</sup>H NMR) spectrum in CDCl<sub>3</sub> solvent revealed various peaks: a singlet at 1.25 ppm (corresponding to 12 hydrogen atoms on positions 3-5 of the pi-piperidine ring), a triplet at 1.66 ppm (corresponding to 8 hydrogen atoms on positions 2 and 6 of the piperidine ring), a doublet at 3.13 ppm

(corresponding to 1 hydrogen atom labeled H- $\beta$ ), a doublet at 3.52 ppm (corresponding to 1 hydrogen atom labeled H- $\alpha$ ), a singlet at 3.93 ppm (corresponding to 6 hydrogen atoms on methoxy groups), a singlet at 5.27 ppm (corresponding to 2 hydrogen atoms on positions 2 and 6), a singlet at 5.52 ppm (corresponding to 1 hydrogen atom on position 4), a singlet at 6.58 ppm (corresponding to 2 hydrogen atoms on positions 4' and 5' of the aromatic ring), and a singlet at 7.62 ppm (corresponding to 2 hydrogen atoms on positions 2' and 6' of the aromatic ring). The <sup>13</sup>CNMR spectrum (recorded in CDCl<sub>3</sub>) shows the following chemical shifts: 24.1 ppm (C-3 of piperidine), 25.1 ppm (C-5 of piperidine), 26.2 ppm (C-4 of piperidine), 37.1 ppm (C- $\beta$ ), 44.6 ppm (C- $\alpha$ ), 47.5 ppm (C-6 of piperidine), 48.2 ppm (C-2 of piperidine), 56.5 ppm (-OCH<sub>3</sub>), 101.9 ppm (C-4), 108.2 ppm (C-2), 108.3 ppm (C-6), 109.6 ppm (C-2'), 121 ppm (C-4'), 134.8 ppm (C-5' & C-6'), 139.4 ppm (C-1'), 146 ppm (C-1), 148.3 ppm (C-3'), 156.3 ppm (C-3 & C-5), and 187.8 ppm (C = O).

The compound is called 8b' and its chemical name is (1,3-dimorpholin-4-yl-propan-1-one) (3,5-dimethoxy-phenyl)-(1,3-hydroxy-phenyl)-2,3. The substance has a yield of 60% and appears as a yellow powder with a melting point. The compound has a melting point of 253°C and a molecular ion peak at m/z 456 [M<sup>+</sup>]. Its molecular formula is C<sub>25</sub>H<sub>32</sub>N<sub>2</sub>O<sub>6</sub>. In the infrared spectrum, it shows absorption peaks at 3424 cm<sup>-1</sup> (OH) and 1642 cm<sup>-1</sup> (C = O) for the ketone group. The <sup>1</sup>H NMR spectrum (recorded in CDCl<sub>3</sub>) shows signals at 3.01 ppm (singlet, 8H, H-2 and H-6 of the morpholine group), 3.41 ppm (doublet, 1H, H- $\beta$ ), 3.58 ppm (doublet, 1H, H- $\alpha$ ), 3.77 ppm (singlet, 8H, H-3 and H-5 of the morpholine group), 3.97 ppm (singlet, 6H, -OCH<sub>3</sub>), 5.41 ppm (singlet, 2H, H-2 & H-6), 5.59 ppm (singlet, 1H, H-4), 6.62 ppm (singlet, 2H, H-4' & H-5'), and 7.53 ppm (singlet, 2H, H-2' & H-6'). The <sup>13</sup>C NMR spectrum (recorded in CDCl<sub>3</sub>) shows signals at 40.6 ppm (C- $\beta$ ), 44.5 ppm (C-2 and C-6 of the morpholine group), 45.8 ppm (C- $\alpha$ ), 56.6 ppm (-OCH<sub>3</sub>), 65.5 ppm (C-3 and C-5 of the morpholine group), 96.9 ppm (C-4), 101.8 ppm (C-2), 101.9 ppm (C-6), 111.2 ppm (C-2'), 114.3 ppm (C-4'), 134.3 ppm (C-5' & C-6'), 138.9 ppm (C-1'), 144.7 ppm (C-1), 157 ppm (C-3'), 160.9 ppm (C-3 & C-5), and 188.1 ppm (C = O).

3-ylpropan-1-one, 3-(4-bromophenyl)-1-(3-hydroxyphenyl)-2,3-dipiperidin-1-yl. The substance is a yellow powder with a melting point. The yield of the substance is 56%. The compound was heated to a temperature of 220°C. The mass-to-charge ratio (m/z) was found to be 470, indicating the presence of the molecular ion [M<sup>+</sup>]. The molecular formula of the compound is C<sub>25</sub>H<sub>31</sub>BrN<sub>2</sub>O<sub>2</sub>. In the infrared spectrum, peaks were observed at 3447 cm<sup>-1</sup>, corresponding to the hydroxyl group (OH), and at 1656 cm<sup>-1</sup>, indicating the presence of a ketone group (C = O). The proton nuclear magnetic resonance (<sup>1</sup>H NMR) spectrum in CDCl<sub>3</sub> solvent showed peaks at 1.25 ppm (singlet) for 12 hydrogen atoms (H-2, H-3, H-5, and H-6) in the piperidine moiety, at 1.73 ppm (triplet) for 8 hydrogen atoms (H-2 and H-6) in the piperidine moiety, at 4.37 ppm (singlet) for 1 hydrogen atom (H- $\beta$ ), at 4.38 ppm (singlet) for 1 hydrogen atom (H- $\alpha$ ), at 7.47 ppm (doublet) for 2 hydrogen atoms (H-2 and H-6) with

a coupling constant (J) of 8.40 Hz, at 7.51 ppm (doublet) for 2 hydrogen atoms (H-3 and H-5) with a coupling constant (J) of 8.40 Hz, at 7.49 ppm (doublet) for 1 hydrogen atom (H-4'), at 7.67 ppm (triplet) for 1 hydrogen atom (H-5'), at 7.74 ppm (singlet) for 1 hydrogen atom (H-2'), and at 7.85 ppm (doublet) for 1 hydrogen atom (H-6'). The <sup>13</sup>CNMR spectrum (CDCl<sub>3</sub>) shows the following chemical shifts: 24.3 ppm (C-3 for piperidine), 25.4 ppm (C-5 for piperidine), 26.4 ppm (C-4 for piperidine), 37.1 ppm (C- $\beta$ ), 44.6 ppm (C- $\alpha$ ), 47.1 ppm (C-6 for piperidine), 47.6 ppm (C-2 for piperidine), 118.1 ppm (C-2'), 122.9 ppm (C-4'), 131.4 ppm (C-2 & C-6), 131.5 ppm (C-3 & C-5), 131.9 ppm (C-6'), 132.2 ppm (C-4), 134.1 ppm (C-5'), 135.1 ppm (C-1), 135.2 ppm (C-1'), 149.3 ppm (C-3'), 193.7 ppm (C = O).

The compound is 1-(4-Bromo-phenyl)-3-(3-hydroxyphenyl)-2,3-di-morpholin-4-yl-propan-1-one. The powder is yellow-orange in color and has a yield of 62%. It has a melting point (m.p.) The compound has a melting point of 245°C and a molecular ion peak at m/z 574 [M<sup>+</sup>]. Its molecular formula is C<sub>23</sub>H<sub>27</sub>BrN<sub>2</sub>O<sub>4</sub>. In the infrared spectrum, it shows absorption bands at 3442 cm<sup>-1</sup> (corresponding to the hydroxyl group) and 1651 cm<sup>-1</sup> (indicating the presence of a ketone group). The <sup>1</sup>H nuclear magnetic resonance spectrum in CDCl<sub>3</sub> solvent reveals signals at  $\delta$  2.59 (singlet, 8H, corresponding to H-2 and H-6 of the morpholine group), 3.77 (singlet, 8H, corresponding to H-3 and H-5 of the morpholine group), 4.27 (singlet, 1H, H- $\beta$ ), 4.47 (singlet, 1H, H- $\alpha$ ), 6.05 (singlet, 2H, H-2 and H-4), 7.51 (doublet, 2H, J = 8.50 Hz, H-3' and H-5'), 7.59 (triplet, 1H, H-5), 7.70 (doublet, 2H, J = 8.50 Hz, H-2' and H-6'), and 7.72 (doublet, 1H, H-6) ppm. The <sup>13</sup>CNMR spectrum of the compound in CDCl<sub>3</sub> shows peaks at the following chemical shifts: 40.4 ppm (C- $\beta$ ), 43.6 ppm (C-2 and C-6 for morpholine), 46.6 ppm (C- $\alpha$ ), 64.6 ppm (C-3 and C-5 for morpholine), 111.4 ppm (C-2 & C-4), 111.8 ppm (C-6), 112.1 ppm (C-4'), 129.1 ppm (C-2' & C-6'), 131.2 ppm (C-3' & C-5'), 134.8 ppm (C-5), 137.8 ppm (C-1'), 39.6 ppm (C-1), 159.5 ppm (C-3), and 185.1 ppm (C = O).

Derivatives of 2-amino-4,6-diphenyl-nicotinonitrile (9a, c, e) were synthesized. Chalcones 3a, c, and f (10 mmol), malononitrile (10 mmol), and ammonium acetate (80 mmol) were combined in 50 milliliters of ethanol using a five-hour reflux heating method. The solid product was separated using filtration, then subjected to an ethanol rinse, drying, and recrystallization in order to get derivatives 9a-c of 2-amino-4,6-diphenyl nicotinonitrile.

The compound 2-Amino-6-(3-roxypropyl)-4-(3-nitropropyl)-nicotinonitrile is denoted as 9a. The yield is 48%, and the substance obtained is a dark powder with a melting point (m.p.). The compound has a melting point of 286°C and a molecular ion peak at m/z 332 [M<sup>+</sup>]. Its molecular formula is C<sub>18</sub>H<sub>12</sub>N<sub>4</sub>O<sub>3</sub>. The infrared spectrum shows absorption bands at 3440 cm<sup>-1</sup> (OH), 3253 cm<sup>-1</sup> and 3357 cm<sup>-1</sup> (NH<sub>2</sub>), 2216 cm<sup>-1</sup> (CN), and 1653 cm<sup>-1</sup> (C = N). The <sup>1</sup>H NMR spectrum (in CDCl<sub>3</sub>) displays signals at  $\delta$  6.96 (multiplet, 4H, H-5, H-2', H-4', H-6'), 7.07 (singlet, 2H, NH<sub>2</sub>), 7.32 (triplet, 1H, H-5'), 7.83 (triplet, 1H, H-5''), 8.11 (doublet, 1H, H-6''), 8.36 (doublet, 1H, H-4''), 8.46 (singlet,

1H, H-2"), and 9.79 (singlet, 1H, -OH) ppm. The <sup>13</sup>C NMR spectrum (in CDCl<sub>3</sub>) shows signals at δ 93.9 (C-3), 114.5 (C-4'), 114.9 (C-5), 115.7 (C-2'), 117.7 (CN), 118.4 (C-6'), 122.6 (C-2''), 123.3 (C-4''), 129 (C-5''), 129.5 (C-5'), 134.5 (C-6''), 137.7 (C-1''), 138 (C-1'), 147 (C-3''), 149.4 (C-4), 153.2 (C-3'), 156.6 (C-6), and 171.7 (C-2) ppm.

The compound is called Nicotinonitrile (9c) and its chemical structure is 2-Amino-4-(4-bromo-phenyl)-6-(3-hydroxy-phenyl). The substance is a powder with a yellow-green color. It has a yield of 30% and a melting point. The compound was heated to a temperature of 250°C. The mass-to-charge ratio (m/z) was found to be 395, indicating the presence of the molecular ion [M<sup>+</sup>]. The molecular formula of the compound is C<sub>18</sub>H<sub>12</sub>BrN<sub>3</sub>O. The infrared (IR) spectrum showed absorption peaks at 3431 cm<sup>-1</sup> (OH), 3226 cm<sup>-1</sup> and 3335 cm<sup>-1</sup> (NH<sub>2</sub>), 2216 cm<sup>-1</sup> (CN), and 1653 cm<sup>-1</sup> (C = N). The <sup>1</sup>H nuclear magnetic resonance (NMR) spectrum, recorded in CDCl<sub>3</sub> solvent, displayed peaks at δ 6.88 (d, 1H, H-6'), 7.05 (s, 2H, NH<sub>2</sub>), 7.18 (s, 1H, H-2'), 7.28 (t, 1H, H-5'), 7.51 (s, 1H, H-5), 7.53 (d, 1H, H-4'), 7.64 (d, 2H, J = 9.00 Hz, H-2" & 6"), 7.77 (d, 2H, J = 9.00 Hz, H-3" & 5"), and 9.63 (s, 1H, OH) ppm. The chemical shifts of the carbon atoms in the compound are as follows: δ85.8 (C-3), 108.7 (C-2'), 113.6 (C-5), 116.4 (CN), 116.7 (C-4'), 117.7 (C-6'), 122.7 (C-4''), 129.1 (C-5''), 130.1 (C-2" & C-6''), 131.3 (C-3" & C-5''), 135.4 (C-1''), 138.4 (C-1'), 152.9 (C-4), 157.2 (C-3'), 158.5 (C-6), 160.3 (C-2) ppm.

### III RESULTS AND DISCUSSION

In this study, we outline the process of esterification involving specific chalcone derivatives and fatty acids, resulting in the synthesis of novel fatty acid chalcone esters (5b-e) and (6b-e). We synthesized chalcone precursors (3a-e) by performing Claisen Schmidt condensation on certain acetophenones (1a-c) and benzaldehydes (2a-d) using established methods described in the literature (Scheme 1) [5,11,12]. The experimental part offers comprehensive depictions of the conditions and procedures. Following the production of these recently developed chalcone derivatives, they were subjected to esterification using stearic or palmitic chlorides, resulting in the synthesis of the desired fatty acid chalcone esters. The stearic/palmitic acid and thionyl chloride (SOCl<sub>2</sub>) were employed to produce the stearyl/palmitoyl chlorides, using the established procedures described in reference [11]. The chalcones (3b-e) were treated dropwise with stearyl/palmitoyl chlorides in pyridine, using dimethylaminopyridine (DMAP) as a base [7,13,14]. The compounds (5b-e) and (6b-e) were successfully synthesized with high yields, as depicted in Scheme 2. These compounds are (E)-3-(3-(substituted phenyl)acryloyl)phenyl/(E)-3-(3-(substituted phenyl)-3-oxoprop-1-en-1-yl)phenyl palmitate and (E)-3-(3-(substituted phenyl)acryloyl)phenyl/(E)-3-(3-(substituted phenyl)-3-oxoprop-1-en-1-yl)phenyl stearate, respectively. The structures of compounds (5b-e) and (6b-e) were verified using a combination of IR and <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy. The previously acquired chalcones (3a-c) were subjected to an electrophilic addition process using bromine in chloroform to produce the corresponding 2,3-dibromo chalcones (7b-d) (Scheme 3). The chemical structures of the

produced compounds (7b-d) were identified and confirmed based on their infrared (IR) and nuclear magnetic resonance (NMR) data. Furthermore, a compound called 2,3-di(morpholin/piperidin-1-yl)substituted-1,3-diphenylpropan-1-one (8b(b')-d) and various other chalcone derivatives with two substituents, either piperidine or morpholine, were effectively synthesized. This was achieved through a nucleophilic substitution reaction of 2,3-dibromo chalcones (7b-d) using either piperidine or morpholine in absolute ethanol. The desired components were identified and purified using column chromatography. Scheme 3 presents the synthesis procedures and reaction conditions for substituted-1,3-diphenylpropan-1-one 5a-c and 2,3-di(morpholin/piperidin-1-yl). The molecular structures of these compounds were ascertained based on the spectrum data obtained from infrared spectroscopy, as well as proton and carbon-13 nuclear magnetic resonance spectroscopy.

Nicotinonitrile derivatives have been synthesized utilizing several synthetic techniques. The synthesis of 2-amino-6-(substituted-phenyl)-4-substitutedphenyl nicotinonitrile (9a,c,e) was achieved by conducting the Michael addition reaction of specific chalcones 3a, c, and e with malonitrile in ethanol, using ammonium acetate as a catalyst (Scheme 4) [15]. The spectral data of these goods confirmed the validity of their structures.

While all chalcone synthesis methods were utilized in this study, some of them did not yield any results. For example, the compounds 3a and 3e are incapable of undergoing a chemical reaction with bromine. Additionally, compound 3a does not exhibit any reactivity towards fatty acids. These can be ascribed to the different substituents present in derivatives of chalcones. This section assessed the antioxidant reactivity of all the synthesized compounds by spectrophotometrically measuring their ability to reduce 2,2-diphenylpicrylhydrazyl (DPPH), a commonly used radical scavenger.

Table 1 displays a comparative assessment of these activities. Compounds (5d-e and 6d-e) that had a para electron-withdrawing substituent, such as a nitro group on the A ring, and/or a meta ester group on the B ring, showed highly favorable activity, as indicated by the results in Table 1. Specifically, compounds 5e and 6e, as depicted in Figure 1, demonstrated the greatest level of inhibition, predominantly at a concentration of C = 2 µg/ml. Significantly, particularly at low concentrations, the activity levels of these compounds are very comparable to that of ascorbic acid. The decrease in activity at higher doses may be attributed to the steric hindrance caused by the long alkyl group chain and the large size of the DPPH molecule. Figure 2 illustrates that compounds (5b and 6b) containing a meta electron-withdrawing ester group on A and a meta-donating methoxy group on B ring exhibited significant inhibition, but to a lesser extent than ascorbic acid. Nevertheless, this behavior aligns with the results of Murti et al.'s research on the production and antioxidant characteristics of several chalcones and flavonoids [9].

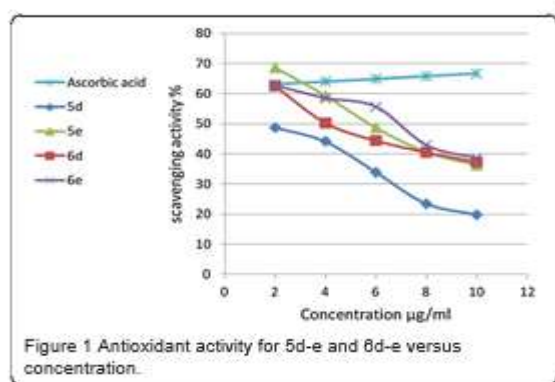


Figure 1 Antioxidant activity for 5d-e and 6d-e versus concentration.

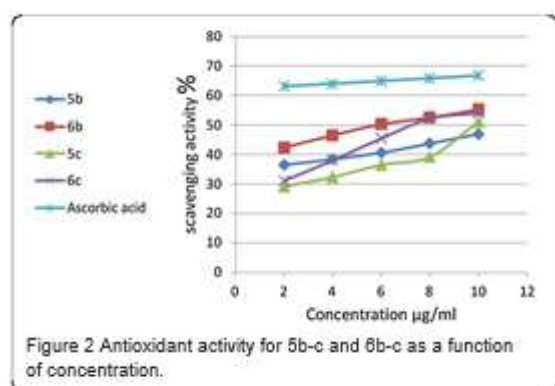


Figure 2 Antioxidant activity for 5b-c and 6b-c as a function of concentration.

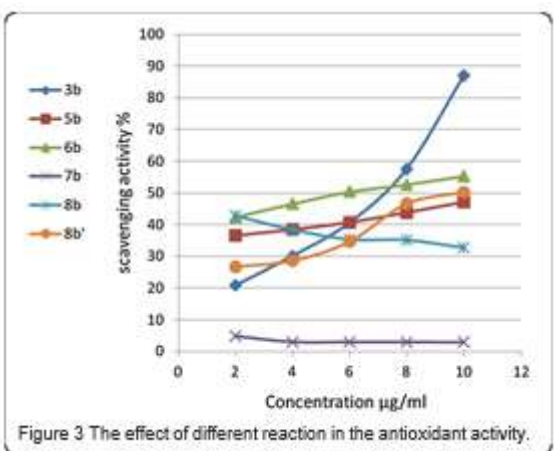


Figure 3 The effect of different reaction in the antioxidant activity.

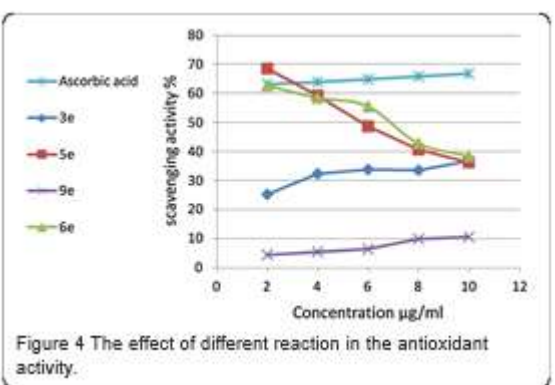


Figure 4 The effect of different reaction in the antioxidant activity.

important additional factor that affects its antioxidant effectiveness. Figures 1 and 2 show that the antioxidant activity of the majority of synthesized chalcone derivatives (except 5c at C = 2 µg/ml) is higher than those with palmitate ester. This is attributed to the presence of stearate ester attached to either ring A or B. The results suggest that enhancing the antioxidant reactivity of the initial chalcones may rely heavily on the arrangement of the hydroxyl group attached to ring A or B [7,8,10]. We assessed the effects of compounds 7b-d and 8b(b')-d, which were produced through addition reactions on these double bonds, to examine their influence on the antioxidant activity of chalcone. Prior studies have shown that the electrophilic addition process in chalcone derivatives, which have different substituents, might lead to a decrease in the antioxidant activity of these derivatives. Consistent with this finding, we noted that the addition of bromine to chalcone compound 3c to form compound 7c resulted in a significant decrease in its activity, dropping from 43.67% to 6.44%, particularly at doses of 2 µg/ml. Surprisingly, when piperidine is used instead of bromine, as in compound 8c, the antioxidant activity is greatly enhanced, leading to a maximum inhibition of 34.82% at a concentration of 2 µg/ml. According to the overall findings, it can be deduced that the presence of a double bond in the chalcone structure is also crucial for improving the antioxidant activity [14,15]. Compound 9c, specifically 2-amino-6-(substituted-phenyl)-4-substituted phenyl nicotinonitrile, was found to contain pyridine rings, cyano groups, and amino groups. These components led to a significant decrease in inhibition compared to the parent chalcone 3e, specifically from 43.67% to 12.06% [13,16-18].

Figures 3 and 4 illustrate the overall effect of the changes made to the chalcone derivatives on DPPH's ability to remove free radicals. As an illustration, the chalcone 3b, which is a parent compound, demonstrates a scavenging activity of 86.94% at a concentration of 10 µg/ml, as depicted in Figure 3. The addition of bromine to its double bond reduces its antioxidant activity to 2.82%. However, when morpholine or piperidine is substituted, the antioxidant activity increases to 32.72% and 50.25% respectively. Nevertheless, the substitution of a fatty acid for a hydroxyl group in rings A or B had a relatively minor impact on the anti-oxidant activity, resulting in a reduction of only 47.02% and 55.42%, respectively.

Compound 5e, a fatty acid substitution for the hydroxyl group in chalcone compound 3e, demonstrates superior antioxidant activity compared to ascorbic acid. This is particularly evident at a concentration of C = 2 µg/ml, where the antioxidant activity jumps from 25.26% to 68.58%. Compound 6e exhibited an activity value of 62.71%, which closely resembled that of ascorbic acid. However, the condensation of chemical 9e (malonitrile) results in a significant decrease in this value, dropping to 21.9%, as depicted in Figure 4. The overall findings of this recent study on chalcone-based fatty acid esters' antioxidant activity revealed the presence of multiple highly potent novel compounds that surpass the effectiveness of commonly used antioxidants such as ascorbic acid. Furthermore, these

The composition of the fatty acid portion of a molecule is an

carefully analyzed research on the activity of structures have offered new insights and reasoning for understanding the role and impact of various functional groups linked to chalcone.

#### IV CONCLUSION

This study successfully synthesized a distinct range of compounds, namely 2-amino-6-(substituted-phenyl)-4-substituted phenyl nicotinonitrile, 2,3-disubstituted chalcones, and chalcone fatty acid esters. The previous group of compounds was synthesized by esterification processes involving chalcones and fatty acid chlorides (namely palmitoyl or stearoyl). Disubstituted analogues were produced using Michael addition and electrophilic addition. The compounds were purified using column chromatography or recrystallization, using the appropriate solvent. The synthesized compounds exhibited synthetic yields ranging from 40 to 90%, and their structures were determined using spectrum data (IR, NMR, MS). Finally, the DPPH technique was employed to assess the antioxidant activity of each synthesized molecule. Chalcone fatty acid esters exhibited favorable efficacy, with certain compounds demonstrating higher antioxidant activity compared to ascorbic acid.

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