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# Nano-Assisted Synthesis And Structural Characterization Of Chalcone Derivatives

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The study investigates the synthesis of six different derivatives of chalcone using silver nanoparticles as a catalyst. Chalcones, known for their wide range of pharmacological activities, can be chemically modified to enhance their biological properties. Silver nanoparticles (AgNPs) have emerged as efficient catalysts due to their high surface area and unique electronic properties. In the present case the AgNPs were synthesized using Green synthesis method and then utilized to catalyze the Claisen-Schmidt Condensation reaction for hydroxyl, methyl, chloride, nitro and methoxy chalcone derivatives. The reaction conditions, including temperature, solvent, and time, were optimized to achieve maximum yield and selectivity. The synthesized different derivatives were characterized using elemental analysis, spectroscopic techniques such as NMR, IR, and UV-Vis spectroscopy, along with mass spectrometry. The catalytic efficiency of AgNPs was compared with conventional catalysts, demonstrating a significant improvement in reaction rate and product purity. This study presents a novel, eco-friendly approach to synthesizing different derivatives of chalcone, highlighting the potential of silver nanoparticles in organic synthesis.

**Keywords:** Chalcone, chalcone-derivatives, green synthesis, elemental analysis, spectroscopic analysis, etc.

## Introduction

Chalcones are organic compounds that belong to the flavonoid family. They have the core structure of 1,3-diphenyl-2-propen-1-one, consisting of two aromatic rings connected by a three-carbon α, β-unsaturated carbonyl system [1-5]. This structure is crucial for their chemical reactivity and biological activity.

The structure of Chalcone includes two aromatic rings (phenyl groups) that can have various substituents, leading to a wide range of chalcone derivatives. The synthesis is simple via the Claisen-Schmidt condensation reaction, which involves the reaction of an aromatic aldehyde with an aromatic ketone in the presence of a base (NaOH in present study). Chalcones are typically light yellow to orange crystalline solids exhibiting a range of physical properties depending on the substituents on the aromatic rings. Chalcones are known for their diverse pharmacological activities, including anti-inflammatory, antimicrobial, antioxidant, anticancer properties [6-11]. Their biological activity is attributed to the presence of the α, β-unsaturated carbonyl group, which can interact with various biological targets. These are used as intermediates in the synthesis of other flavonoids and heterocyclic compounds.

**Materials and Method**

Several chalcone derivatives are relatively easy to synthesize, especially those with simple substituents on the aromatic rings. In the present study six different derivatives viz. hydroxy, methyl, dihydroxy, chloride, nitro and methoxy were synthesised using Claisen-Schmidt Condensation reaction. The reaction conditions, including temperature, solvent, and time, were optimized to achieve maximum yield and selectivity [12-21]. The reaction were performed twice (one without the catalyst and second with AgNPs as the catalyst). Figure 1 shows the basic structure of the synthesised chalcone and the different chemical reactions involved are shown in Figure 1. The name of the different derivatives obtained is given in Table 1. The reactant 1 for all the synthesis is acetophenone. The details of reactant 2 are also given in Table 1.

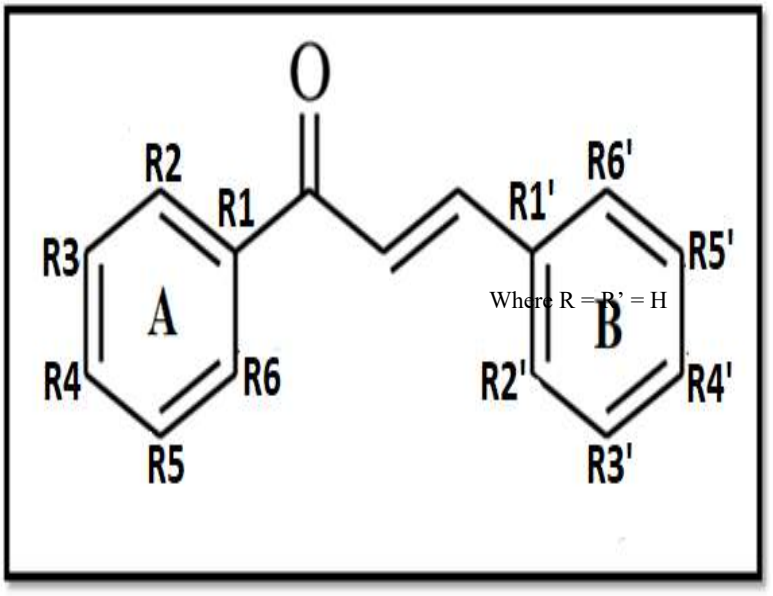


Figure 1: Structure of Chalcone

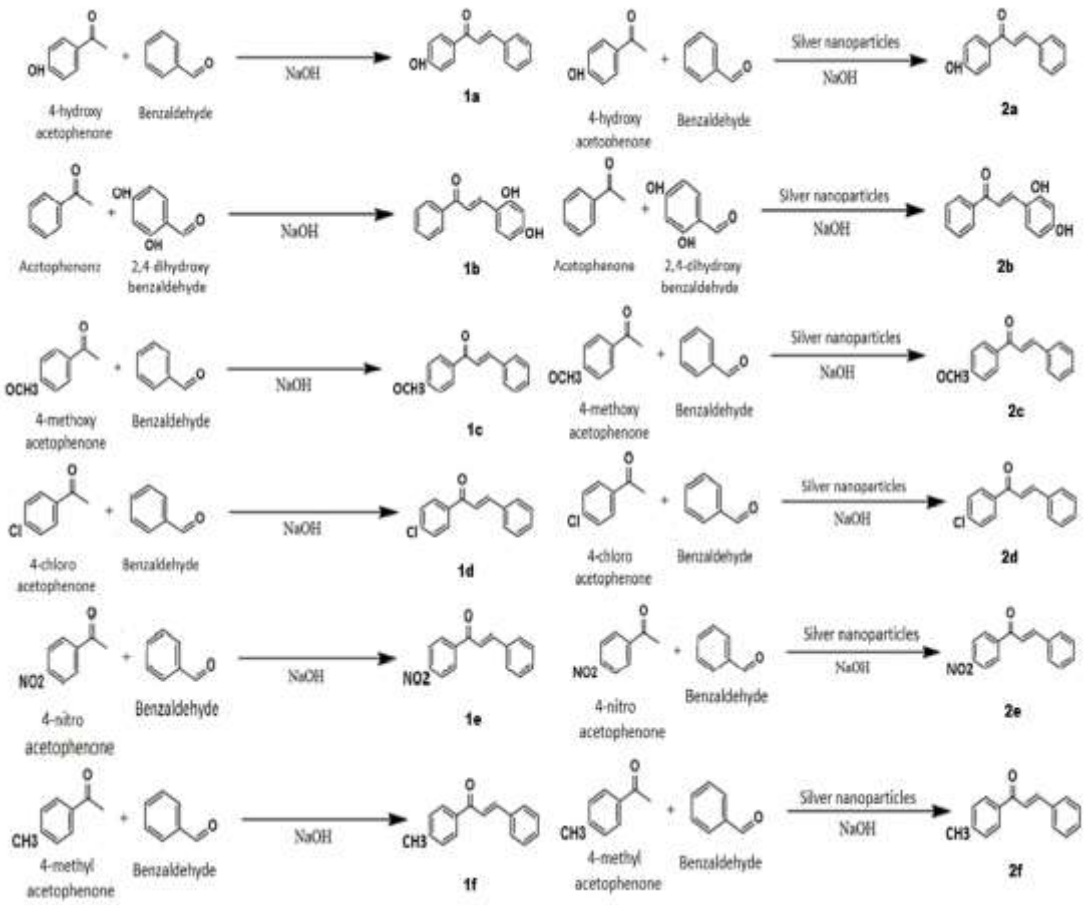


Figure 2: Different chemical reactions for synthesising chalcone derivatives with and without the presence of catalyst.

Table 1: Details of the synthesized chalcone derivatives

| Sr. No. | Reactant 2 | Compound Code | Compound Name | IUPAC Nomenclature |
|---|---|---|---|---|
| 1 | Benzaldehyde | -- | Chalcone | (2E)-1,3-diphenyl-2-propen-1-one |
| 2 | 4-hydroxybenzaldehyde | 1a | 4’-hydroxychalcone | (E)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one |
| 3 | 2,4-dihydroxybenzaldehyde | 1b | 2’,4’-dihydroxychalcone | (E)-1-(2,4-dihydroxyphenyl)- |

| | | | | |
|---|---|---|---|---|
| | | | | 3-phenylprop-2-en-1-one |
| 4 | 4-methoxybenzaldehyde | 1c | 4'-methoxychalcone | (E)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one |
| 5 | 4-chlorobenzaldehyde | 1d | 4-chlorochalcone | (2E)-3-(4-chlorophenyl)-1-phenylprop-2-en-1-one |
| 6 | 4-nitrobenzaldehyde | 1e | 4-nitrochalcone | (2E)-3-(4-nitrophenyl)-1-phenylprop-2-en-1-one |
| 7 | 4-Methylbenzaldehyde | 1f | 4-methylchalcone | (2E)-3-(4-methylphenyl)-1-phenylprop-2-en-1-one |
| 8 | 4-hydroxybenzaldehyde | 2a | 2',4'-dihydroxychalcone | (E)-1-(2,4-dihydroxyphenyl)-3-phenylprop-2-en-1-one |
| 9 | 2,4-dihydroxybenzaldehyde | 2b | 4'-methoxychalcone | (E)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one |
| 10 | 4-methoxybenzaldehyde | 2c | 2',4'-dihydroxychalcone | (E)-1-(2,4-hydroxyphenyl)-3-phenylprop-2-en-1-one |
| 11 | 4-chlorobenzaldehyde | 2d | 4-chlorochalcone | (2E)-3-(4-chlorophenyl)-1-phenylprop-2-en-1-one |
| 12 | 4-nitrobenzaldehyde | 2e | 4-nitrochalcone | (2E)-3-(4-nitrophenyl)-1-phenylprop-2-en-1-one |
| 13 | 4-Methylbenzaldehyde | 2f | 4-methylchalcone | (2E)-3-(4-methylphenyl)-1-phenylprop-2-en-1-one |

## Results and Discussion

The physical properties and elemental analysis of synthesised chalcone derivatives were performed and calculated. Table 2 shows the results for all the 12 derivatives obtained.

Table 2: Physical properties and elemental analysis of synthesised chalcone derivatives

| **Sr. no.** | **Compound** | **Molecular formula** | **Molar mass** | **Melting Point ($^0$C)** | **Percentage yield (%)** | **Elemental Analysis** | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | **Theoretical** | | | **Experimental** | | |
| | | | | | | **C %** | **H %** | **O %** | **C %** | **H %** | **O %** |
| **1** | Chalcone | $C_{15}H_{12}O$ | 208 | 56 | 80.42 | 86.54 | 5.76 | 7.7 | 86.51 | 5.77 | 7.72 |
| **2** | 1a | $C_{15}H_{14}O_2$ | 224 | 181 | 76.64 | 80.36 | 2.36 | 17.28 | 80.38 | 2.35 | 17.27 |
| **3** | 1b | $C_{15}H_{12}O_3$ | 240 | 142 | 76.66 | 75 | 5 | 20 | 75 | 5 | 20 |
| **4** | 1c | $C_{16}H_{14}O_2$ | 238 | 107 | 78.43 | 80.67 | 5.89 | 13.44 | 80.64 | 5.9 | 13.46 |
| **5** | 1d | $C_{15}H_{11}ClO$ | 242.5 | 114 | 75.98 | 73.23 | 4.53 | 6.59 | 73.2 | 4.55 | 6.6 |
| **6** | 1e | $C_{15}H_{13}NO_3$ | 253 | 165 | 77.61 | 71.15 | 4.35 | 18.97 | 71.18 | 4.34 | 18.95 |
| **7** | 1f | $C_{16}H_{14}O$ | 222 | 57 | 74.28 | 86.49 | 6.3 | 7.21 | 86.55 | 6.28 | 7.17 |
| **8** | 2a | $C_{15}H_{14}O_2$ | 224 | 182 | 88.73 | 80.36 | 2.36 | 17.28 | 80.38 | 2.35 | 17.27 |
| **9** | 2b | $C_{15}H_{12}O_3$ | 240 | 142 | 89.12 | 75 | 5 | 20 | 75.1 | 4.98 | 19.97 |
| **10** | 2c | $C_{16}H_{14}O_2$ | 238 | 106 | 86.74 | 80.67 | 5.89 | 13.44 | 80.63 | 5.9 | 13.47 |
| **11** | 2d | $C_{15}H_{11}ClO$ | 242.5 | 115 | 86.88 | 73.23 | 4.53 | 6.59 | 73.2 | 4.54 | 6.61 |
| **12** | 2e | $C_{15}H_{13}NO_3$ | 253 | 165 | 83.75 | 71.15 | 4.35 | 18.97 | 71.18 | 4.33 | 18.98 |
| **13** | 2f | $C_{16}H_{14}O$ | 222 | 57 | 87.64 | 86.49 | 6.3 | 7.21 | 86.45 | 6.31 | 7.24 |

The different spectral analysis for all the compounds is given below:

**Compound Chalcone:-** (2E)-1,3-diphenyl-2-propen-1-one
IR (ν max) cm-1 3084 (OH), 1642 (C=O), 1577, 1496 (ring C=C),
MS m/z: 208 ($M^+$)
1 H NMR- δ 8.27, δ 8.13, δ 7.27, δ 6.89, δ 4.13, δ 2.50, δ 2.35, δ 1.43.

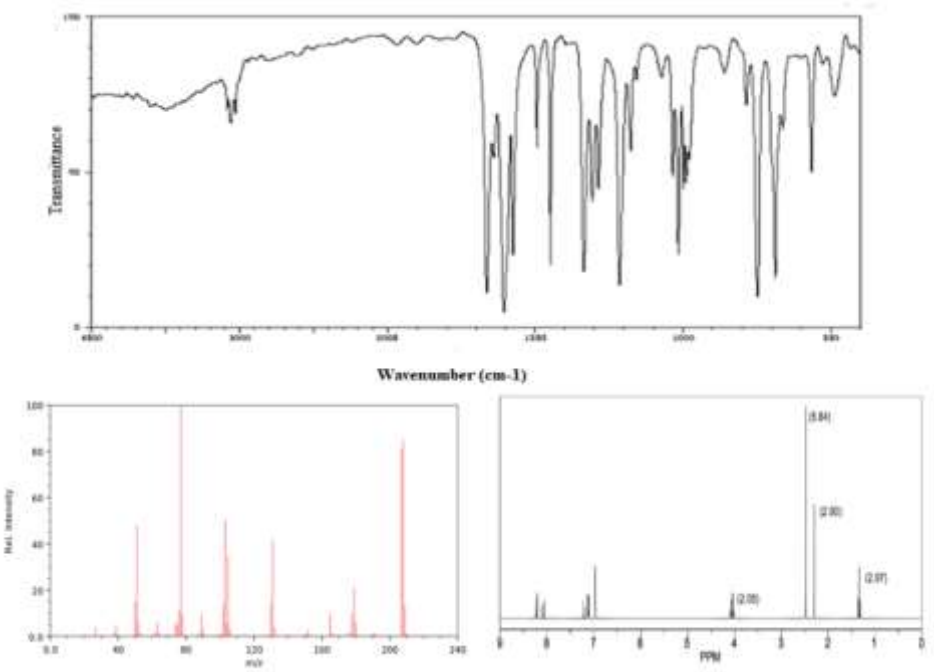


Figure 3: FTIR, Mass spectra and NMR spectra of Chalcone

**Compound a :-** (E)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one
IR (ν max) cm-1 3133 (OH), 1646 (C=O), 1514, 1495 (ring C=C),
MS m/z: 224 ($M^+$)
1 H NMR- δ 8.27, δ 7.75, δ 7.61, δ 6.89,

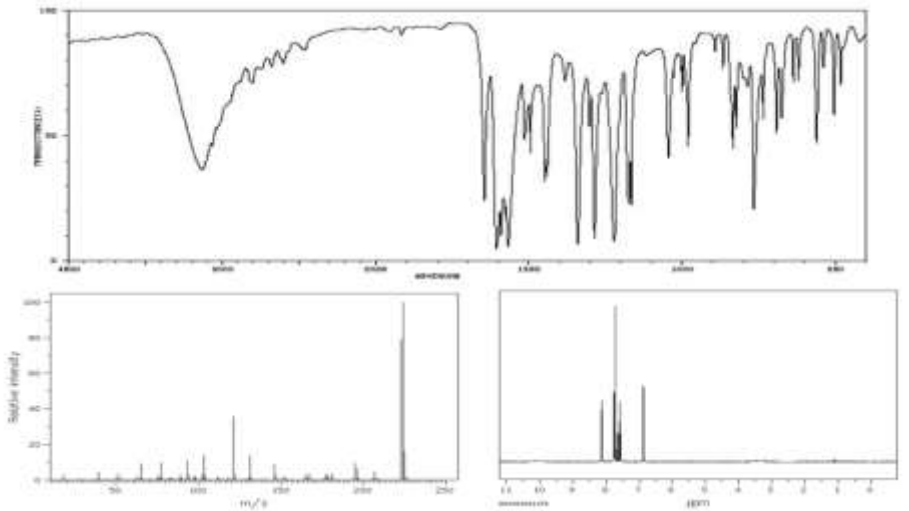

Figure 4: FTIR, Mass spectra and NMR spectra of 4'-hydroxyhalcone
**Compound b:-** (E)-1-(2,4-hydroxyphenyl)-3-phenylprop-2-en-1-one

IR (ν max) cm-1 3074 (OH), 1604 (C=O), 1440 (ring C=C),
MS m/z: 240 ($M^+$)
1 H NMR- δ 8.06, δ 7.96, δ 7.60, δ 7.40, δ 7.33, δ 6.45, δ 6.38, δ 5.35.

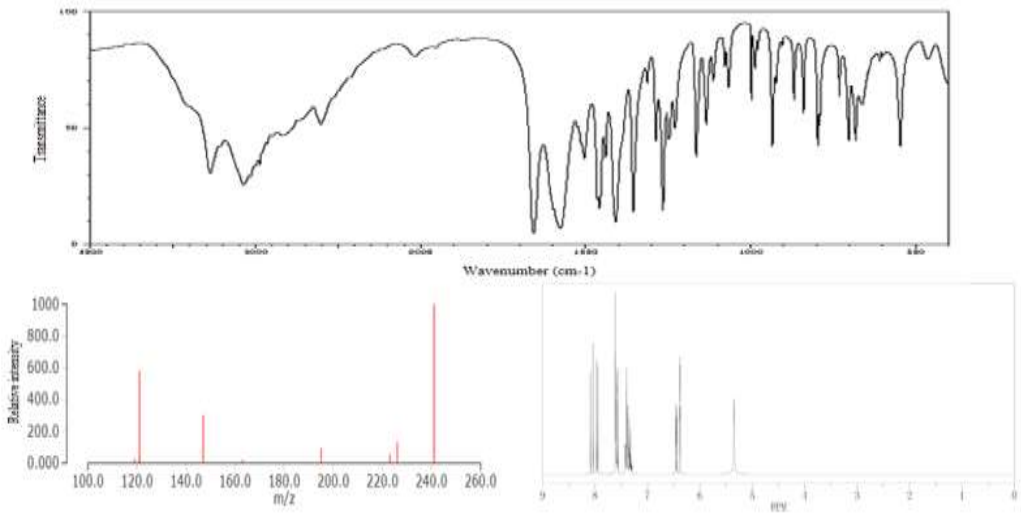


Figure 5: FTIR, Mass spectra and NMR spectra of 2'4'- dihydroxchalcone

**Compound c :-** (E)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one
IR (ν max) cm-1 3068 (OH), 1656 (C=O), 1511, 1496 (ring C=C),
MS m/z: 238 ($M^+$)
1 H NMR- δ 8.20, δ 7.78, δ 7.55, δ 7.42, δ 7.00, δ 3.92

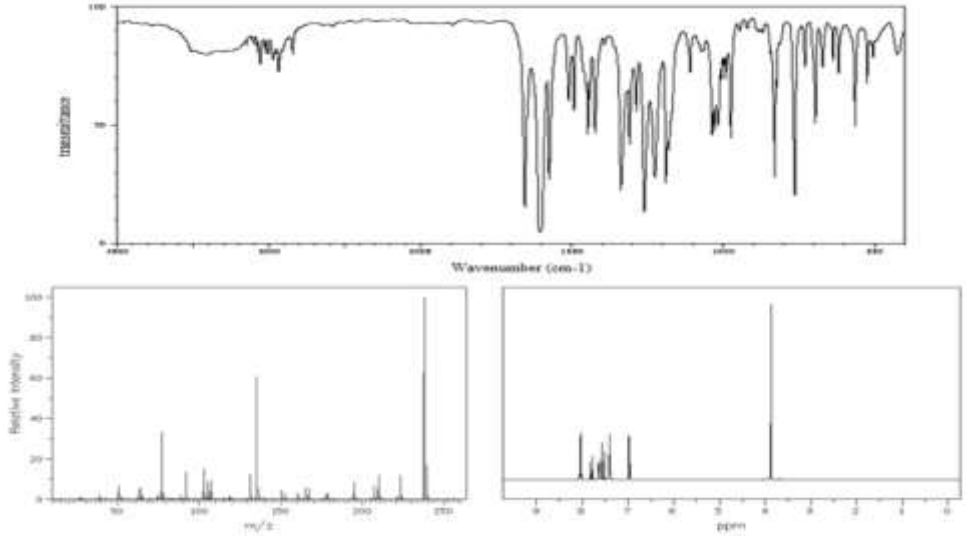


Figure 6: FTIR, Mass spectra and NMR spectra of 4'- methoxychalcone
**Compound d :-** (2E)-3-(4-chlorophenyl)-1-phenylprop-2-en-1-one
IR (ν max) cm-1 3068 (OH), 1567 (C=O), 1448 (ring C=C),

MS m/z: 242.5 ($M^+$)
1 H NMR- δ 7.89, δ 7.86, δ 7.78, δ 7.73, δ 7.66, δ 7.63, δ 7.58, δ 7.56, δ 7.47, δ 7.41, δ 7.40, δ 7.38.

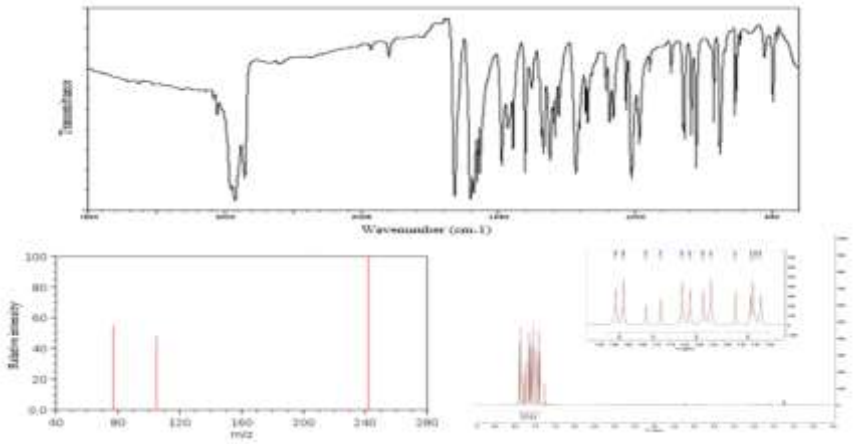

Figure 7: FTIR, Mass spectra and NMR spectra of 4-chlorochalcone

**Compound e :-** (2E)-3-(4-nitrophenyl)-1-phenylprop-2-en-1-one
IR (ν max) cm-1 3077 (OH), 1576 (C=O), 1488 (ring C=C),
MS m/z: 222 ($M^+$)
1 H NMR- δ 8.21, δ 8.20, δ 8.03, δ 7.89, δ 7.88, δ 7.64, δ 7.73.

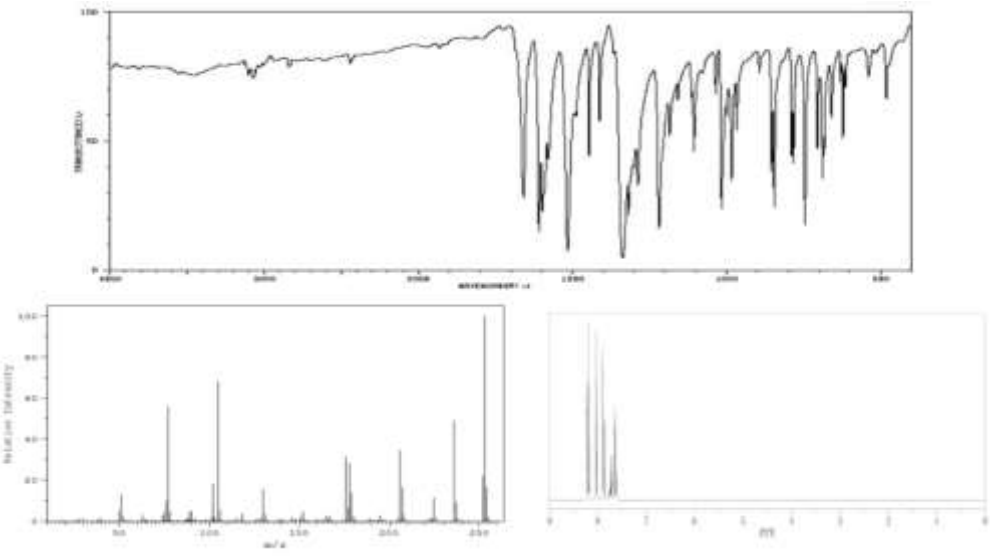

Figure 8: FTIR, Mass spectra and NMR spectra of 4-nitroChalcone
The table 2 gives the elemental analysis for the all the different derivatives of chalcones and the figures 3 - 8 shows the FTIR, Mass and NMR spectra for the different chalcone derivatives. From the results it is clearly seen that the percentage yield of the derivates using silver nano particles is high in comparison to the derivatives formed without catalyst.

## Conclusion

The study investigates the synthesis of six different derivatives of chalcone using silver nanoparticles as a catalyst and a set of derivatives without the catalyst. The results clearly indicate that the yield of all the derivatives of chalcone is more in case were silver nano particles as catalyst. The different spectral analysis obtained for the different compounds also indicates that the product obtained is in the purest form. The calculated and obtained elemental analysis for all the compounds are in agreement. Thus the study presents a novel, eco-friendly approach to synthesizing different derivatives of chalcone, highlighting the potential of silver nanoparticles in organic synthesis.

## References


(1) Okolo, E. N.; Ugwu, D. I.; Ezema, B. E.; Ndefo, J. C.; Eze, F. U.; Ezema, C. G.; Ezugwu, J. A.; Ujam, O. T. New chalcone derivatives as potential antimicrobial and antioxidant agent. Scientific Reports. 2021, 11, 21871.

(2) Nurkenov, O.; Ibraev, M.; Schepetkin, I.; Khlebnikov, A.; Seilkhanov, T.; Arinova, A.; Isabaeva, M. Synthesis, structure, and anti-inflammatory activity of functionally substituted chalcones and their derivatives. Russian Journal of General Chemistry. 2019, 89 (7), 1360−1367.

(3) Higgs, J.; Wasowski, C.; Marcos, A.; Jukic,ˇ M.; Paván, C. H.; Gobec, S.; de Tezanos Pinto, F.; Colettis, N.; Marder, M. Chalcone derivatives: synthesis, in vitro and in vivo evaluation of their anti-anxiety, anti-depression and analgesic effects. Heliyon. 2019, 5 (3), e01376.

(4) Murtaza, S.; Mir, K. Z.; Tatheer, A.; Ullah, R. S. Synthesis and evaluation of chalcone and its derivatives as potential anticholinergic agents. Letters in Drug Design & Discovery. 2019, 16 (3), 322−332.

(5) Al Zahrani, N. A.; El-Shishtawy, R. M.; Elaasser, M. M.; Asiri, A. M. Synthesis of novel chalcone-based phenothiazine derivatives as antioxidant and anticancer agents. Molecules. 2020, 25 (19), 4566.

(6) Welday Kahssay, S.; Hailu, G. S.; Taye Desta, K. Design, Synthesis, Characterization and in vivo Antidiabetic Activity Evaluation of Some Chalcone Derivatives. Drug Design, Development and Therapy. 2021, 15, 3119.

(7) Jain, A.; Jain, D. Synthesis, characterization and biological evaluation of some new heterocyclic derivatives of chalcone as antihyperglycemic agents. Int. J. Pharmaceutical Sci. Res. 2019, 59, 5700−5706.

(8) Aljohani, G.; Al-Sheikh Ali, A.; Alraqa, S. Y.; Itri Amran, S.; Basar, N. Synthesis, molecular docking and biochemical analysis of aminoalkylated naphthalene-based chalcones as acetylcholinesterase inhibitors. Journal of Taibah University for Science. 2021, 15 (1), 781− 797.

(9) SG, P.; Patil, N.; Patil, S. M.; Bhusange, A.; Ravindranath, S. Synthesis, Characterization, Antimicrobial studies and Evaluation of Stability constants of Cu (II), Ni (II) and Co (II) complexes with the ligands derived from chalcone derivatives. Appl. Organomet. Chem. 2022, 36 (2), e6465.

(10) Wang, J.; Huang, L.; Cheng, C.; Li, G.; Xie, J.; Shen, M.; Chen, Q.; Li, W.; He, W.; Qiu, P.; et al. Design, synthesis and biological evaluation of chalcone analogues with novel dual antioxidant mechanisms as potential anti-ischemic stroke agents. Acta Pharmaceutica Sinica B 2019, 9 (2), 335−350.

(11) Han, X.; Peng, B.; Xiao, B.-B.; Cao, S.-L.; Yang, C.-R.; Wang, W.-Z.; Wang, F.-C.; Li, H.-Y.; Yuan, X.-L.; Shi, R.; et al. Synthesis and evaluation of chalcone analogues containing a 4-oxoquinazolin-2-yl group as potential anti-tumor agents. Eur. J. Med. Chem. 2019, 162, 586−601.

(12) Chen, Z.; Li, P.; Hu, D.; Dong, L.; Pan, J.; Luo, L.; Zhang, W.; Xue, W.; Jin, L.; Song, B. Synthesis, antiviral activity, and 3D-QSAR study of novel chalcone derivatives containing malonate and pyridine moieties. Arabian Journal of Chemistry. 2019, 12 (8), 2685−2696.

(13) Ayman, M.; El-Messery, S. M.; Habib, E. E.; Al-Rashood, S. T.; Almehizia, A. A.; Alkahtani, H. M.; Hassan, G. S. Targeting microbial resistance: Synthesis, antibacterial evaluation, DNA binding and modeling study of new chalcone-based dithiocarbamate derivatives. Bioorganic Chemistry. 2019, 85, 282−292.

(14) Ouyang, Y.; Li, J.; Chen, X.; Fu, X.; Sun, S.; Wu, Q. Chalcone derivatives: role in anticancer therapy. Biomolecules. 2021, 11 (6), 894.

(15) Č izmáriková,ˇM.; Takác,ˇP.; Spengler, G.; Kincses, A.; Nové, M.; Vilková, M.; Mojziš ,J. New chalcone derivative inhibits ABCB1 in multidrug resistant T-cell lymphoma and colon adenocarcinoma cells. Anticancer Res. 2019, 39 (12), 6499−6505.

(16) Duran, N.; Polat, M. F.; Aktas, D. A.; Alagoz, M. A.; Ay, E.; Cimen, F.; Tek, E.; Anil, B.; Burmaoglu, S.; Algul, O. New chalcone derivatives as effective against SARS-CoV-2 agent. Int. J. Clin. Pract. 2021, e14846.

(17) Bhoj, P.; Togre, N.; Bahekar, S.; Goswami, K.; Chandak, H.; Patil, M. Immunomodulatory Activity of Sulfonamide Chalcone Compounds in Mice Infected with Filarial Parasite, Brugia malayi. Indian Journal of Clinical Biochemistry 2019, 34 (2), 225−229.

(18) Reddy, M. R.; Aidhen, I. S.; Reddy, U. A.; Reddy, G. B.; Ingle, K.; Mukhopadhyay, S. Synthesis of 4-C-β-D-Glucosylated Isoliquiritigenin and Analogues for Aldose Reductase Inhibition Studies. Eur. J. Org. Chem. 2019, (24), 3937−3948.

(19) Shah, U.; Patel, S.; Patel, M.; Gandhi, K.; Patel, A. Identification of chalcone derivatives as putative non-steroidal aromatase inhibitors potentially useful against breast cancer by molecular docking and ADME prediction. Indian J. Chem. 2020, B59, 283−293.

(20) Kim, H.-G.; Oh, H.-J.; Ko, J.-H.; Song, H. S.; Lee, Y.-G.; Kang, S. C.; Lee, D. Y.; Baek, N.-I. Lanceoleins AG, hydroxychalcones, from the flowers of Coreopsis lanceolata and their chemopreventive effects against human colon cancer cells. Bioorganic Chemistry. 2019, 85, 274−281.

(21) Henry, E. J.; Bird, S. J.; Gowland, P.; Collins, M.; Cassella, J. P. Ferrocenyl chalcone derivatives as possible antimicrobial agents. Journal of antibiotics. 2020, 73 (5), 299−308.