



SYNTHESIS, CHARACTERIZATION, AND BIOLOGICAL EVALUATION OF CYANO AND CHLORO BENZALDEHYDE DERIVATIVES OF FLUORINATED CHALCONES

Sandip U Agare^a, Sanjay Tajane^b, Tanuja V Kadre^{a*}

ABSTRACT

The approaches outline the synthesis of a new series of chalcone using cyano- and chloro-substituted benzaldehydes and 4-fluoro-3-methylacetophenone. The structure of the produced compounds was characterized using elemental analysis and spectral (¹H NMR, FT-IR, and UV) methods. *In vitro* testing was done on the substances that had antibacterial and antifungal activities. All the compounds displayed good binding affinities with the target microorganism proteins, although compounds **H** and **I** displayed the strongest affinities, according to molecular docking. The synthesized compounds in vitro antimicrobial activity against *Escherichia coli* (MCC 2412), *Staphylococcus aureus* (MCC 2408), *Bacillus subtilis* (MCC 2010), *Pseudomonas aeruginosa* (MCC 2080), *Saccharomyces cerevisiae* (MCC 1033), and *Candida albicans* (MCC 1439) was examined using the discs diffusion method. The yeast *Candida albicans* was the target of antifungal action in substances.

Keywords: 4-Fluoro-3-methylacetophenone, dichlorobenzaldehyde, trichlorobenzaldehyde, antibacterial activity, antifungal activity.

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INTRODUCTION:

Chalcones are flavonoid-class phenolic phytochemicals that are produced through the shikimate pathway. The biosynthesis of flavonoids can be traced back to chalcones. In terms of chemistry, chalcones are generally two-ring ketones joined by an alkenone unit with three carbons. However, some dihydrochalcones, or saturated ketones, might also fit this description¹. The alkenone unit in these ketones is three carbons instead of one. Naturally occurring chalcones are consistently found to have one or more phenolic hydroxyl functionalities as well as phenyl and geranyl substitutions on the aromatic rings. Many of the thousands of naturally occurring chalcones that have been reported in the literature² have been demonstrated to interact with different biomolecules and to have modulatory and cytoprotective qualities. There are numerous patents covering the properties of chalcones and their derivatives, including their anticancer, anti-inflammatory, antimutagenic, antioxidant, and cytotoxic properties³. Due to the structural simplicity and potential therapeutic applications of chalcone derivatives, a number of bioinspired syntheses and assessments of their bioactivities have been reported in the literature⁴.

The natural product with a therapeutic use that contains a chalcone scaffold. Chalcones are abundant in nature and relatively easy to synthesize, giving them a special place in medicinal chemistry. Since the 1800s, numerous scientists have created synthetic chalcones. Nonetheless, it is widely acknowledged that Kostanecki and Tambor were the first to effectively treat *o*-acetoxychalcone dibromides with alcoholic alkali in order to create synthetic chalcones⁵. However, the core chalcone nucleus is produced by the present methods of chalcone synthesis of two aromatic ring molecules, such as acetophenone and benzaldehyde, using an alkaline base and a polar solvent⁶⁻⁸. Chalcone is synthesized by numerous researchers using unconventional methods, including solvent-free, ultrasonic, microwave, grinding, etc⁹⁻¹². These methods save energy, prevent dangerous chemicals and environmental hazards, lessen wastewater pollution, save the environment, preserve

biological life, and save time, which makes them extremely significant in today's world.

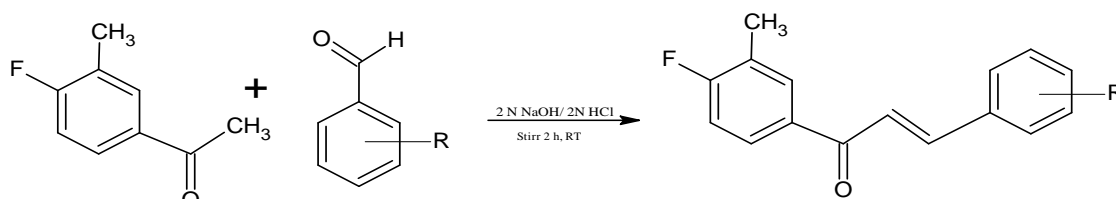
The effective method for preparing a number of structurally intriguing chalcone derivatives is described here. a base-catalyzed condensation process between cyano- and chloro-substituted benzaldehydes and 4-fluoro-3-methylacetophenone to create a number of unique chalcone derivatives that can be ground using solvent-free, ultrasonic, and chemical methods. To further develop effective and less dangerous antibacterial drugs, they are tested against Gram-positive (*Bacillus subtilis* MCC 2010 and *Staphylococcus aureus* MCC 2408) and Gram-negative (*E. coli* MCC 2412 and *Pseudomonas aeruginosa* MCC 2080) bacteria.

EXPERIMENTAL METHOD:

High-purity synthetic chemical reagents and solvents from commercial sources were used in this investigation. The solvents were dried or purified using accepted techniques. To determine the uncorrected melting points of the synthesized compounds, open capillary tubes were utilized. Using silica gel as the stationary phase and pet ether and ethyl acetate as the mobile phases, TLC was utilized to confirm the progress of the reaction and the product's conversion. The characteristics of each spot were visible under ultraviolet light. A Bruker 400 MHz spectrometer and a Bruker FT-IR spectrometer were used to record the ¹H NMR and IR spectra, respectively.

SYNTHESIS OF CHALCONES:

Chalcone synthesis is based on the Claisen-Schmidt condensation reaction. NaOH (2 mol) was added to a solution of 4-fluoro-3-methylacetophenone (2 mmol) and substituted cyano- and chloro-substituted benzaldehydes (2 mmol) in ethanol (10mL). Up until full conversion, the mixture was agitated at room temperature. Following the reaction's completion, the mixture was neutralized at 0 °C with dil. HCl and the chalcone were separated via filtration. Alcohol was used to recrystallize the crude chalcone, purifying it to produce (A-I).



Scheme 1

2-[(1E)-3-(4-fluoro-3-methylphenyl)-3-oxoprop-1-en-1-yl]benzonitrile (A),

White solid, yield = 76.62%; m. p. 163°C. FT-IR (KBr) cm^{-1} : 3178 (Ar-CH₃), 2815 (-CH=), 3110 (C-CH₃), 2227 (-CN), 1655 (C=O, chalcone), 1582/1479 (C=C), 1242 (C-F), 741 (Tri. Sub benz. Ring), 654 (di. Sub benz ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.368 (s, 3H, CH₃), 7.098 (d, 1H, -CH= (*J* = 14.18), 7.142-7.394 (td, 2H, Ar C-H (*J* = 8.73, 0.53), 7.490-7.529 (dd, 1H, Ar C-H (*J* = 1.89, 0.53), 7.705-7.440 (dd, 1H, 7.630 (dd, 1H, -CH= (*J* = 15.03), Ar C-H (*J* = 8.70, 1.78), 7.867-7.923 (ddd, 2H, Ar C-H (*J* = 7.90, 1.90, 1.10). Anal. calcd for C₁₇H₁₂FNO: C, 76.97; H, 4.56; F, 7.16; O, 6.03.

3-[(1E)-3-(4-fluoro-3-methylphenyl)-3-oxoprop-1-en-1-yl]benzonitrile (B),

White solid, yield = 74.72%; m. p. 176°C. FT-IR (KBr) cm^{-1} : 3071 (Ar-CH₃), 2932 (-CH=), 3029 (C-CH₃), 2229 (-CN), 1669 (C=O, chalcone), 1585/1478 (C=C), 1225 (C-F), 759 (Tri. Sub benz. Ring), 672 (di. Sub benz ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.346-2.406 (s, 3H, CH₃), 7.362-7.188 (d, 1H, -CH= (*J* = 14.67), 7.568-7.734 (td, 2H, Ar C-H (*J* = 8.70, 0.45), 7.768-7.807 (dd, 1H, -CH= (*J* = 14.66), 7.807-7.786 (dd, 1H, Ar C-H (*J* = 1.88, 0.54), 7.886-7.887 (ddd, 1H, Ar C-H (*J* = 8.00, 1.69, 1.10), 7.890-7.892 (dd, 1H, Ar C-H (*J* = 8.66, 1.93), 7.938-7.939 (ddd, 1H, Ar C-H (*J* = 7.97, 1.93, 1.17), 7.956-7.968 (ddd, 1H, Ar C-H (*J* = 1.93, 1.71, 0.77). Anal. calcd for C₁₇H₁₂FNO: C, 76.97; H, 4.56; F, 7.16; O, 6.03.

4-[(1E)-3-(4-fluoro-3-methylphenyl)-3-oxoprop-1-en-1-yl]benzonitrile (C),

White solid, yield = 85.66%; m. p. 178°C. FT-IR (KBr) cm^{-1} : 3061 (Ar-CH₃), 2921 (-CH=), 3003 (C-CH₃), 2225 (-CN), 1662 (C=O, chalcone), 1594/1447 (C=C), 1239 (C-F), 755 (Tri. Sub benz. Ring), 677 (di. Sub benz ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.339-2.397 (s, 3H, CH₃), 7.137-7.297 (d, 1H, -CH= (*J* = 16.11), 7.460-7.617 (dd, 1H, Ar C-H (*J* = 8.69, 0.54), 7.603-7.627 (dd, 1H, -CH= (*J* = 1.89, 0.55), 7.706-7.779 (ddd, 2H, Ar C-H (*J* = 8.45, 1.75, 0.48), 7.818-7.900 (dd, 1H, Ar C-H (*J* = 8.75, 1.89, 7.908-7.947 (ddd, 2H, Ar C-H (*J* = 8.49, 1.69, 0.48). Anal. calcd for C₁₇H₁₂FNO: C, 76.97; H, 4.56; F, 7.16; O, 6.03.

(2E)-3-(2, 3-dichlorophenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one (D),

White solid, yield = 71.52%; m. p. 193°C. FT-IR (KBr) cm^{-1} : 3062 (Ar-CH₃), 2924 (-CH=), 3009 (C-CH₃), 1667 (C=O, chalcone), 1592/1450 (C=C), 1251 (C-F), 860 (C-Cl), 675 (Tri. Sub benz. Ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.345 (s, 3H,

CH₃), 7.032-7.115 (d, 1H, -CH= (*J* = 15.72), 7.287-7.306 (dd, 1H, Ar C-H (*J* = 8.74, 0.55), 7.428-7.540 (dd, 2H, Ar C-H (*J* = 7.93, 1.24), 7.626-7.676 (dd, 1H, Ar C-H (*J* = 7.93, 7.57), 7.865-7.886 (dd, 1H, Ar C-H (*J* = 1.86, 0.55), 7.893-7.910 (d, -CH= (*J* = 15.72), 7.928-7.910 (dd, 2H, Ar C-H (*J* = 1.89, 0.55). Anal. calcd for C₁₆H₁₁Cl₂FO: C, 62.16; H, 3.59; Cl: 22.93, F, 6.15; O, 5.18.

(2E)-3-(2, 4-dichlorophenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one (E),

White solid, yield = 82.85%; m. p. 188°C. FT-IR (KBr) cm^{-1} : 3095 (Ar-CH₃), 2925 (-CH=), 3061 (C-CH₃), 1610 (C=O, chalcone), 1581/1465 (C=C), 1237 (C-F), 863 (C-Cl), 719 (Tri. Sub benz. Ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.338 (s, 3H, CH₃), 7.038-7.167 (d, 1H, -CH= (*J* = 15.71), 7.293-7.345 (dd, 1H, Ar C-H (*J* = 8.74, 0.55), 7.446-7.500 (dd, 2H, Ar C-H (*J* = 8.26, 0.52), 7.666-7.724 (dd, 1H, Ar C-H (*J* = 1.77, 0.52), 7.837-7.873 (dd, 1H, Ar C-H (*J* = 8.26, 1.77), 7.879-7.894 (d, -CH= (*J* = 15.71), 7.899-7.915 (dd, 1H, Ar C-H (*J* = 1.89, 0.55), 7.929-8.135 (dd, 1H, Ar C-H (*J* = 8.74, 1.89). Anal. calcd for C₁₆H₁₁Cl₂FO: C, 62.16; H, 3.59; Cl: 22.93, F, 6.15; O, 5.18.

(2E)-3-(2, 5-dichlorophenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one (F),

White solid, yield = 75.40%; m. p. 183°C. FT-IR (KBr) cm^{-1} : 3085 (Ar-CH₃), 2926 (-CH=), 3065 (C-CH₃), 1668 (C=O, chalcone), 1585/1438 (C=C), 1257 (C-F), 853 (C-Cl), 669 (Tri. Sub benz. Ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.371 (s, 3H, CH₃), 7.110-7.155 (d, 1H, -CH= (*J* = 15.72), 7.229-7.294 (dd, 1H, Ar C-H (*J* = 8.74, 0.55), 7.269-7.393 (dd, 1H, Ar C-H (*J* = 8.06, 1.75), 7.404-7.666 (dd, 1H, Ar C-H (*J* = 8.06, 0.51), 7.818-7.867 (dd, 1H, Ar C-H (*J* = 1.89, 0.55), 7.835-7.867 (d, -CH= (*J* = 15.72), 7.875-7.880 (dd, 1H, Ar C-H (*J* = 8.74, 1.89), 7.901-7.936 (dd, 1H, Ar C-H (*J* = 1.75, 0.51). Anal. calcd for C₁₆H₁₁Cl₂FO: C, 62.16; H, 3.59; Cl: 22.93, F, 6.15; O, 5.18.

(2E)-3-(2, 6-dichlorophenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one (G),

White solid, yield = 79.61%; m. p. 178°C. FT-IR (KBr) cm^{-1} : 3116 (Ar-CH₃), 2977 (-CH=), 3061 (C-CH₃), 1665 (C=O, chalcone), 1592/1424 (C=C), 1257 (C-F), 853 (C-Cl), 669 (Tri. Sub benz. Ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.371 (s, 3H, CH₃), 7.110-7.155 (d, 1H, -CH= (*J* = 15.72), 7.229-7.294 (dd, 1H, Ar C-H (*J* = 8.74, 0.55), 7.269-7.393 (dd, 1H, Ar C-H (*J* = 8.06, 1.75), 7.404-7.666 (dd, 1H, Ar C-H (*J* = 8.06, 0.51), 7.818-7.867 (dd, 1H, Ar C-H (*J* = 1.89, 0.55), 7.835-7.867 (d, -CH= (*J* = 15.72), 7.875-7.880 (dd, 1H, Ar C-H (*J* = 8.74,

1.89), 7.901-7.936 (*dd*, 1H, Ar C-H ($J = 1.75, 0.51$)). Anal. calcd for $C_{16}H_{11}Cl_2FO$: C, 62.16; H, 3.59; Cl: 22.93, F, 6.15; O, 5.18.

(2E)-3-(3, 4-dichlorophenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one (H),

White solid, yield = 77.35%; m. p. 175°C. FT-IR (KBr) cm^{-1} : 3371 (Ar-CH₃), 2926 (-CH=), 3071 (C-CH₃), 1665 (C=O, chalcone), 1585/1417 (C=C), 1246 (C-F), 847 (C-Cl), 686 (Tri. Sub benz. Ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.403-2.411 (*s*, 3H, CH₃), 7.042-7.136 (*d*, 1H, -CH= ($J = 15.70$), 7.425-7.430 (*dd*, 1H, Ar C-H ($J = 8.74, 0.55$), 7.434-7.530 (*dd*, 1H, Ar C-H ($J = 8.02, 1.89$), 7.535-7.663 (*dd*, 1H, Ar C-H ($J = 1.89, 0.55$), 7.702-7.905 (*dd*, 1H, Ar C-H ($J = 8.02, 0.52$), 7.919-7.923 (*dd*, 1H, Ar C-H ($J = 1.89, 0.52$), 7.927-7.942 (*d*, -CH= ($J = 15.70$), 7.945-7.946 (*dd*, 1H, Ar C-H ($J = 8.74, 1.89$). Anal. calcd for $C_{16}H_{11}Cl_2FO$: C, 62.16; H, 3.59; Cl: 22.93, F, 6.15; O, 5.18.

(2E)-3-(2, 3, 5-dichlorophenyl)-1-(4-fluoro-3-methylphenyl)prop-2-en-1-one (I),

White solid, yield = 80.02%; m. p. 188°C. FT-IR (KBr) cm^{-1} : 3071 (Ar-CH₃), 2924 (-CH=), 2958 (C-CH₃), 1679 (C=O, chalcone), 1586/1498 (C=C), 1248 (C-F), 858 (C-Cl), 673 (Tri. Sub benz. Ring). ¹H NMR (400 MHz, CDCl₃, δ ppm): 2.387 (*s*, 3H, CH₃), 7.112-7.133 (*d*, 2H, -CH= ($J = 15.57$), 7.294-7.416 (*ddd*, 3H, Ar C-H ($J = 8.74, 0.55, 8.23$), 7.424-7.534 (*dd*, 1H, Ar C-H ($J = 1.89, 0.55$), 7.748-7.757 (*dd*, 1H, Ar C-H ($J = 8.02, 0.52$), 7.902-7.934 (*dd*, 2H, Ar C-H ($J = 8.74, 1.89$). Anal. calcd for $C_{16}H_{10}Cl_3FO$: C, 55.93; H, 2.93; Cl: 30.99, F, 5.53; O, 4.66.

DISC-DIFFUSION METHOD:

Discs of Whatman's filter paper no. 1 with a diameter of 6 mm were used in the disc diffusion method¹³ to assess the antibacterial activity of azomethine. The chalcones solution was prepared at a concentration of 1000 ppm. Each sterile petri dish was filled with 20 mL of sterile growth media (nutrient agar), sealed, and allowed to solidify in order to cultivate the bacteria. Following a 48-hour incubation period, disc diffusion studies¹⁴⁻¹⁵ were conducted on the microorganism broth cultures. The sample, control, and standard discs were air-dried at room temperature to get rid of any solvent residue that might have tampered with the results after they had been sterilized and infected. In order to maximize the diffusion of chemicals from the test disc into the agar plate, the plates were kept at a low temperature for one hour following a 48-hour incubation period at 37 °C for the bacterium¹⁶.

RESULTS AND DISCUSSION:

Chalcones (A-I) were synthesized by the Claisen-Schmidt condensation of 4-fluoro-3-methylacetophenone with cyano- and chloro-substituted benzaldehydes in the presence of sodium hydroxide²⁴. With the aid of sodium hydroxide, a basic catalyst, 4-fluoro-3-methylacetophenone, and cyano- and chloro-substituted benzaldehydes were combined to create the chalcones derivatives of the moiety shown in **Scheme 1** at an equimolar concentration. Because they are resistant to different organic solvents, non-hygroscopic, and insoluble in water, all chalcone compounds are stable at room temperature. The structures of all newly synthesized compounds were verified by data from the IR, NMR, and UV-visible spectra.

FT-IR SPECTRA:

The infrared frequencies exhibited by the cyano- and chloro-substituted benzaldehydes derivatives of 4-fluoro-3-methylacetophenone are summarized in the experimental section. For 4-fluoro-3-methylacetophenone derivatives, a moderately intense band was observed, which corresponded to the aromatic α (C-H) frequency range. The new chalcones showed weak broadband in the 2958–3071 cm^{-1} range because of an aromatic (-CH₃) group²⁵. The developed new derivatives' FTIR spectra display bands at 2912–2977 cm^{-1} that are linked to the stretching vibration of -CH=. All chalcone compounds have a strong band in their infrared spectra, at 1610–1679 cm^{-1} , which is caused by the ν (C=O) group²⁶⁻²⁷. The medium intensity band between 1581-1594 cm^{-1} and 1417-1498 cm^{-1} is caused by the aromatic (C=C) vibrations. The (C-F) band was found in 4-fluoro-3-methylacetophenone derivatives with benzaldehyde substituents at about 1217–1277 cm^{-1} . The medium intensity band appeared at 853-863 cm^{-1} due to the presence of the C-Cl stretching vibration.

¹H-NMR Spectra:

The protons of the methyl group are assigned to singlets (2.377-2.379 ppm) in the ¹H-NMR spectra of compounds A-I. The presence of two doublets with characteristic coupling constants (J) of 15.57-15.72 Hz in the range 6.811-6.701 and 7.541-7.596 ppm in the ¹H NMR spectra of all the synthesized chalcones²⁹ confirmed the generation of chalcones. New chalcones that are synthesized exhibit a multiplet peak at 7.139-8.390 ppm integrating for the aromatic proton³⁰.

ANTIBACTERIAL ACTIVITY:

The disc diffusion method of antimicrobial tests was performed using Gram-positive (*Bacillus subtilis* MCC 2010 and *Staphylococcus aureus* MCC 2408) and Gram-negative (*E. coli* MCC 2412 and *Pseudomonas aeruginosa* MCC 2080) bacterial strains. **Table 1** summarizes the minimum inhibitory concentrations (MICs) of the chalcone derivatives against each of the four bacterial strains. Of the nine heterocyclic chalcones that were investigated, three of them demonstrated notable effectiveness against *E. coli* (MCC 2412). While compounds **A-I** with fluoro substituents on

the phenyl ring showed even more activity against *Bacillus subtilis* (MCC 2010), the traditional medication was also effective against them. All compounds except those having a phenyl moiety (compounds **A-I**) and the reference medication were ineffective against *Pseudomonas aeruginosa* (MCC 2080). The compound's potential for treating drug-resistant bacteria was demonstrated by its antimicrobial efficacy against *Pseudomonas aeruginosa* (MCC 2080). While some compounds with cyano substituents showed moderate or no efficacy against the bacteria, others showed no effect at all³⁰⁻³⁴.

Table 1: Antibacterial studies of **A-I** compounds

Compound	Antibacterial Activity (zone of inhibition)			
	<i>S. aureus</i>	<i>B. subtilis</i>	<i>E. coli</i>	<i>P. aeruginosa</i>
A	10	0	15	14
B	9	0	8	11
C	12	0	8	9
D	8	0	0	12
E	0	0	0	15
F	0	0	0	17
G	9	12	10	14
H	10	13	9	10
I	11	12	8	7
<i>Streptomycin</i>	8	7	6	8

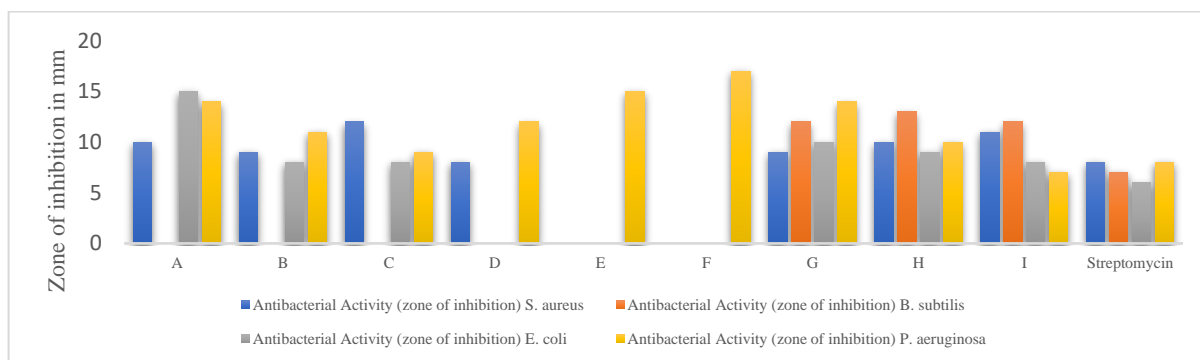


Figure 1: Antibacterial studies of **A-I** compounds

Table 2: Antifungal activities of compounds **A-I**

Compound	Antibacterial Activity (zone of inhibition)	
	<i>C Albican</i>	<i>S. C.</i>
A	11	12
B	7	6
C	10	6
D	6	0
E	7	8
F	10	10
G	6	8
H	10	9
I	9	8
<i>Fluconazole</i>	7	7

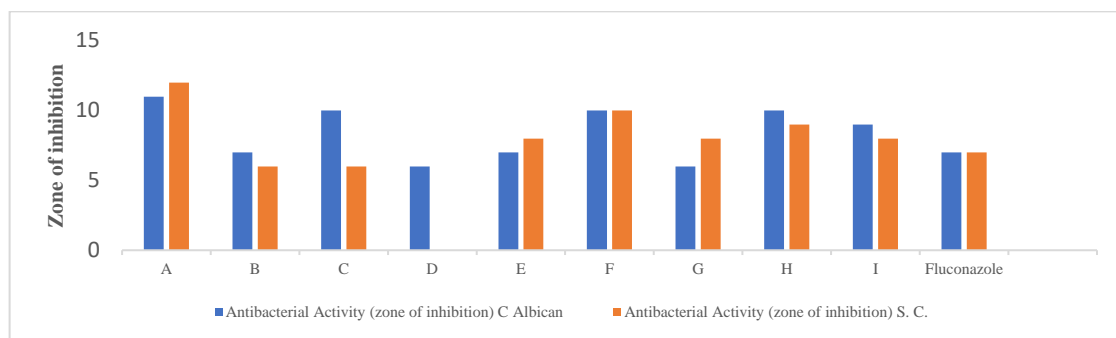


Figure 2: Antifungal activity of compounds A-I

ANTIFUNGAL ACTIVITY:

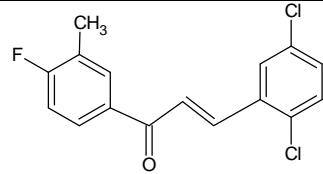
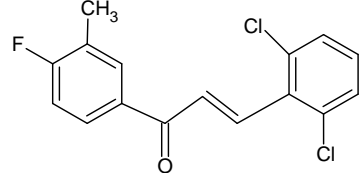
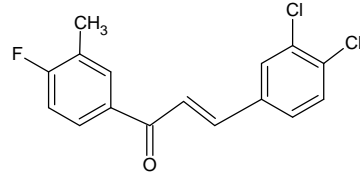
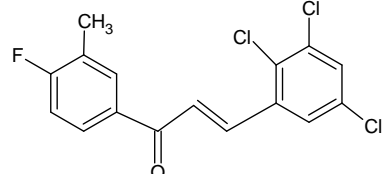
The reference standard in this study was *fluconazole*, which had a MIC of 50 ppm against the tested fungal species. For *Saccharomyces cerevisiae* (MCC1033) and *Candida albicans* (MCC1439), the inhibition zones were 9–11 mm and 6–12 mm, respectively. With a minimum inhibitory concentration (MIC) of 75 µg/mL against *Saccharomyces cerevisiae* (MCC1033) and *Candida albicans* (MCC1439), all compounds tested in **Table 2** demonstrated strong fungicidal potential and were more effective than the reference medication.

CONCLUSION:

The synthesis, characterization, and antibacterial and antifungal activity of 4-fluoro-3-

methylacetophenone derivatives substituted with cyano and chloro-benzaldehyde are reported in this work. FT-IR, UV, and ¹H NMR spectral spectroscopy were used to examine the structures of these compounds. Next, Gram-positive (*Bacillus subtilis* MCC 2010 and *Staphylococcus aureus* MCC 2408) and Gram-negative (*E. coli* MCC 2412 and *Pseudomonas aeruginosa* MCC 2080) bacteria were used to test the antibacterial properties of the fluorinated chalcones (A-I). The compounds showed better antibacterial activity than streptomycin and appeared to be effective against a broad range of bacteria. Compounds H and I serve as a basis for the synthesis of novel antifungal and antibacterial inhibitors based on the binding free energy value.

Comp Code	MW	Formula	MP	Structure
A	265	C ₁₇ H ₁₂ FNO	163	
B	265	C ₁₇ H ₁₂ FNO	176	
C	265	C ₁₇ H ₁₂ FNO	178	
D	309	C ₁₆ H ₁₁ Cl ₂ FO	193	
E	309	C ₁₆ H ₁₁ Cl ₂ FO	188	

F	309	$C_{16}H_{11}Cl_2FO$	183	
G	309	$C_{16}H_{11}Cl_2FO$	178	
H	309	$C_{16}H_{11}Cl_2FO$	175	
I	343	$C_{16}H_{10}Cl_3FO$	188	

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