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Newer chalcone scaffolds with reactive functional groups: Process, spectral and single crystal XRD studies

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ABSTRACT

Chalcones are versatile scaffolds for the synthesis of various heterocyclic systems with commercial utility. This work describes the synthesis of five novel chalcone derivatives. Syntheses were performed by a simple one-pot, straightforward Claisen-Schmidt condensation catalyzed with pyrrolidine and KOH. The chalcones were prepared by condensation of 4-formylbenzonitrile with different aromatic ketones at room temperature. The structures of all compounds have been investigated by FT-IR, NMR, and HR-MS spectroscopy. In addition, one chalcone structure was characterized by single-crystal XRD study. Crystal data for $C_{21}H_{15}NO_2$ (Ch2): monoclinic, space group $P2_1/c$ (no. 14), a = 6.5694(3) Å, b = 33.2697(15) Å, c = 7.4516(4) Å, β = 97.563(2)°, V = 1614.47(14) Å^3, Z = 4, T = 293(2) K, μ(MoKα) = 0.083 mm^{-1}, D_{calc} = 1.289 g/cm^3, 16000 reflections measured (4.898° ≤ 2Θ ≤ 49.99°), 2822 unique (R_{int} = 0.0249, R_{sigma} = 0.0196) which were used in all calculations. The final R_1 was 0.0484 (I > 2σ(I)) and wR_2 was 0.1257 (all data). The absorption maxima of all novel products were evaluated by UV-visible spectroscopy. These well-established structures of all newly prepared chalcone scaffolds with reactive functional groups (*i.e.* nitrile and 2-propenone) can be exploited as a crucial intermediate in the synthesis of new heterocyclic scaffolds with fluorescence and other applications.

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1. Introduction

Chalcones are privileged structures and have been widely used as an effective template in medicinal chemistry for potential drug findings [1,2]. It is a simple, versatile scaffold established from many naturally occurring compounds [3]. Several chalcone derivatives have also been synthesized due to their convenient synthesis [4]. Various natural products and their modified compounds with chalcone skeleton (Figure 1) have shown plentiful exciting biological activities with medical potential against various diseases [5,6]. Chemically, they consist of two aromatic rings joined by a three-carbon, α,β-unsaturated carbonyl system. Their diverse structures allow them to cyclize and produce a variety of heterocyclic compounds with various biological activities [7-9]. Many synthetic equivalents, such as aza-chalcone and chalcone derivatives incorporating isoxazole, pyrazole, and indole, have been developed in recent decades [10]. Antioxidant, anticancer, antibacterial, antiprotozoal, antiulcer, antiviral, antihistaminic, anti-HIV, cytotoxic and anti-inflammatory actions have been demonstrated (Figure 1) in natural and synthesized chalcone derivatives [8-11].

In recent years, chalcone and its derivatives have exhibited numerous other properties, such as optical, photochemical, and nonlinear optic properties (Figure 1), and have been used as fluorescent dyes in light-emitting diodes, fluorescent sensors, and as fluorescent probes [12-16]. Due to its π-conjugated system, the optical characteristics of chalcone and its derivatives have received substantial attention due to their nonlinear optical and fluorescence nature due to the delocalization of the electronic charge and overlapping π-orbitals [17]. Because of their bioactivity and optoelectronic applications, many researchers have recently provoked the multifunctional behavior of chalcones.

The chalcone scaffolds with reactive functional groups can enlarge the importance of the chalcone moiety for its synthetic utility. In this paper, we describe the synthesis of five novel chalcone molecules with a reactive functional group. These molecules were prepared by base-catalyzed Claisen-Schmidt condensation. During this investigation, two different catalysts, pyrrolidine and potassium hydroxide, were studied to develop two different protocols and have comparative studies. The spectral behavior of chalcones is an important key factor in understanding the formation of chalcone.

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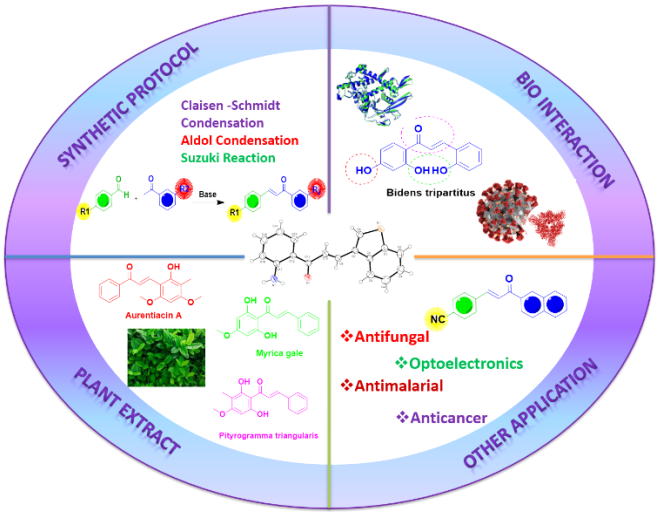
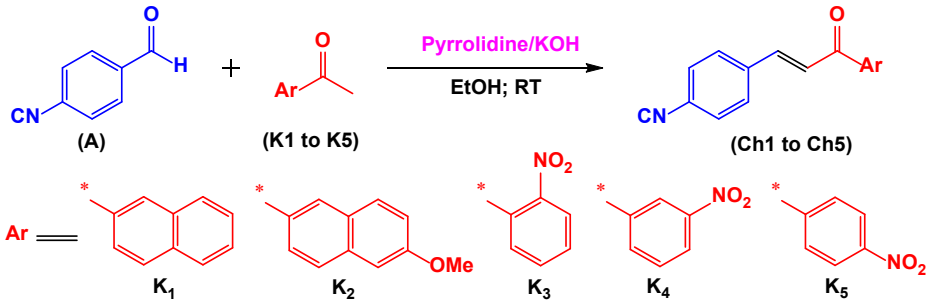


Figure 1. Chalcone: A privileged structure in chemical sciences.



Scheme 1. Synthesis of chalcone from 4-formylbenzonitrile.

All newly prepared chalcones were analyzed by UV-vis, FTIR, and NMR spectroscopy. These chalcone derivatives can be used as a key intermediate for the synthesis of new novel heterocyclic scaffolds.

2. Experimental

2.1. Materials and methods

All required chemicals were obtained from commercial sources and used without further purification. Solvents were dried over molecular sieves if necessary. ^{1}H NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 at room temperature using a Bruker AVANCE III 500 MHz (AV500) multi-nuclei solution NMR spectrometer, TMS was used as internal reference, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, m = multiplet, br = broad, app = apparent), coupling constants (J, Hz), and assignment. ^{13}C and DEPT-135 NMR spectra were measured on a Bruker AVANCE III 125 MHz (AV125) instrument with complete proton decoupling. Chemical shifts in ppm from the residual solvent were reported as an internal standard. Infrared (IR) spectra were recorded neat by ATR on a Thermo Nicolet iS50 FT-IR spectrometer and are reported in cm^{-1}. HR-MS data were obtained in methanol with Thermo Scientific Orbitrap Elite mass spectrometer. The melting point is measured by the open capillary method using a Sigma melting point apparatus. Single-crystal structural data were recorded on Bruker Kappa APEXII. For thin layer chromatography (TLC) analysis throughout this work, Merck precoated TLC plates (silica gel 60GF_{254}, 0.25 mm) were used. The products were purified by recrystallisation or column chromatography on silica gel 60 (Merck, 230-400 mesh).

2.2. General process for pyrrolidine-catalyzed chalcone synthesis

To a stirred solution of 4-formylbenzonitrile (A, 1.62 g, 10 mmol) in ethanol (5 mL), aryl methyl ketone derivatives (K1-K5; 10 mmol) dissolved in ethanol (2-3 mL) were added portion-wise (Scheme 1). The reaction mixture was stirred at room temperature for 20 min, during which time it turned into a homogeneous solution. Then 2 mL of pyrrolidine or 1 mL 0.5 mM KOH was added dropwise and the resulting mixture was stirred at room temperature for 6-8 h and the reaction mixture was neutralized by 0.1-0.2 N HCl where precipitation occurred. The precipitated product of chalcone was then collected by filtration. The crude product was purified by recrystallisation from $CHCl_3$:MeOH (1:1, *v*/*v*, 10 mL) to produce the product (80-85% yield) as yellow to light brown needles (Ch1-Ch5). A single crystal suitable for X-ray diffraction of chalcone was obtained by recrystallization of Ch2 from a saturated solution in DMSO.

(E)-4-(3-(naphthalen-2-yl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch1): Color: Yellow solid. M.p.: 158-160 °C. ^{1}H NMR (500 MHz, DMSO-d_6, δ, ppm): 8.570-8.569 (d, *J* = 0.5 Hz, 1H, Ar-H), 8.137-8.116 (dd, *J* = 8.5, 8.5 Hz, 1H, Ar-H), 8.040-8.025 (d *J* = 7.5 Hz, 1H, Ar-H), 7.995-7.978 (d, *J* = 8.5 Hz, 1H, Ar-H), 7.948-7.931 (d, *J* = 8.5 Hz, 1H, Ar-H), 7.885-7.853 (d, *J* = 16, 1H, α-CH), 7.812-7.794 (m, 2H, Ar-H and β-CH), 7.781 (s, 1H, Ar-H), 7.764-7.747 (dd, *J* = 6.5, 7.0 Hz, 2H, Ar-H), 7.680-7.648 (m, 1H, Ar-H), 7.632-7.599 (m, 1H, Ar-H). ^{13}C NMR (125 MHz, DMSO-d_6, δ, ppm): 189.49 (1C, C=O), 142.02 (1C, CH), 139.30 (1C, Ar-C), 135.70 (1C, Ar-C), 135.00 (1C, Ar-C), 132.72 (1C, Ar-C), 132.53 (1C, Ar-

Table 1. Comparative yield for two different processes.

Compounds	Catalyst and Yield (%)	
	KOH	Pyrrolidine
Ch1	80	82
Ch2	76	79
Ch3	85	86
Ch4	80	83
Ch5	84	86

C), 130.24 (1C, Ar-C), 129.58 (1C, Ar-C), 128.85 (1C, Ar-C), 127.91 (1C, Ar-C), 128.85 (1C, Ar-C), 127.91 (1C, Ar-C), 127.02 (1C, Ar-C), 125.09 (1C, Ar-C), 124.30 (1C, CH), 118.42 (1C, CN), 113.52 (1C, Ar-C). DEPT-135 (125 MHz, DMSO-d_6, δ, ppm): 142.03, 132.72, 130.24, 129.58, 128.85, 128.77, 127.92, 127.02, 125.08, 124.30. HR-MS (EI, *m/z*) calcd. for $C_{20}H_{14}ON$: 284.1067; Found: 284.1070.

(E)-4-(3-(6-methoxynaphthalen-2-yl)-3-oxoprop-1-en-1-yl) benzonitrile (Ch2): Color: Yellow solid. M.p.: 172-174 °C. ^{1}H NMR (500 MHz, DMSO-d_6, δ, ppm): 8.500-8.498 (d *J* = 1 Hz, 1H, Ar-H), 8.114-8.094 (dd, *J* = 8.5, 8.5 Hz, 1H, Ar-H), 7.919-7.901 (d, *J* = 9 Hz, 1H, Ar-H), 7.863-7.858 (d, *J* = 2.5 Hz, 1H, Ar-H), 7.841-7.832 (d, *J* = 4.5 Hz, 1H, Ar-H) 7.800-7.790 (m, 2H, Ar-H, α-CH), 7.780-7.769 (m, 1H, β-CH), 7.748-7.731 (dd, *J* = 6.5, 7 Hz, 2H, Ar-H), 7.265-7.242 (dd, *J* = 9, 9 Hz, 1H, Ar-H), 7.208-7.203 (d, *J* = 2.5 Hz, 1H, Ar-H), 3.986 (s, 3H, CH_3-O). ^{13}C NMR (125 MHz, DMSO-d_6, δ, ppm): 189.01 (1C, C=O), 160.04 (1C, Ar-C), 141.58 (1C, CH), 139.43 (1C, Ar-C), 137.48 (1C, Ar-C), 133.00 (1C, Ar-C), 132.69 (1C, Ar-C), 132.02 (1C, Ar-C), 131.18 (1C, Ar-C), 130.18 (1C, Ar-C), 129.67 (1C, Ar-C), 128.71 (1C, Ar-C), 127.84 (1C, Ar-C), 127.52 (1C, Ar-C), 125.08 (1C, Ar-C), 125.05 (1C, CH), 119.96 (1C, Ar-C), 118.45 (1C, CN), 113.37 (1C, Ar-C), 105.90 (1C, Ar-C), 55.49 (1C, CH3-O). DEPT-135 (125 MHz, DMSO-d_6, δ, ppm): 141.59, 132.69, 131.19, 130.18, 128.72, 127.52, 125.07, 125.06, 119.97, 105.89, 55.49. HR-MS (EI, *m/z*) calcd. for $C_{21}H_{16}O_2N$: 314.1176, Found 314.1176.

(E)-4-(3-(2-nitrophenyl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch3): Color: Yellow solid. M.p.: 156-158 °C. ^{1}H NMR (500 MHz, DMSO-d_6, δ, ppm): 8.241-8.223 (dd, *J* = 8, 8 Hz, 1H, Ar-H), 7.979-7.962 (dd, *J* = 6.5, 7 Hz, 2H, Ar-H), 7.947-7.915 (m, 1H, α-CH), 7.909-7.892 (dd, *J* = 6.5, 7 Hz, 2H, Ar-H), 7.853-7.819 (m, 1H, β-CH), 7.768-7.750 (dd, *J* = 7.5, 8 Hz, 1H, Ar-H), 7.484 (s, 2H, Ar-H). ^{13}C NMR (125 MHz, DMSO-d_6, δ, ppm): 192.57 (1C, C=O), 147.07 (1C, Ar-C), 143.85 (1C, CH), 139.01 (1C, Ar-C), 135.53 (1C, Ar-C), 135.03 (1C, Ar-C), 133.22 (1C, Ar-C), 132.17 (1C, Ar-C), 129.93 (1C, Ar-C), 129.60 (1C, Ar-C), 129.12 (1C, Ar-C), 125.11 (1C, CH), 118.98 (1C, CN), 113.18 (1C, Ar-C). DEPT-135 (125 MHz, DMSO-d_6, δ, ppm): 143.86, 135.04, 133.23, 132.17, 129.93, 129.60, 129.12, 125.12.

(E)-4-(3-(3-nitrophenyl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch4): Color: Yellow solid. M.p.: 126-128 °C. ^{1}H NMR (500 MHz, DMSO-d_6, δ, ppm): 8.874-8.867 (t, 1H, Ar-H), 8.636-8.618 (m, 1H, Ar-H), 8.534-8.511 (m, 1H, α-CH), 8.211-8.180 (d, *J* = 16 Hz, 1H, β-CH), 8.165-8.148 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.971-7.955 (d, *J* = 8 Hz, 2H, Ar-H), 7.918-7.902 (d, *J* = 8 Hz, 1H, Ar-H), 7.892-7.886 (d, *J* = 3 Hz, 1H, Ar-H). ^{13}C NMR (125 MHz, DMSO-d_6, δ, ppm): 188.02 (1C, C=O), 148.74 (1C, Ar-C), 143.63 (1C, CH), 139.43 (1C, Ar-C), 138.86 (1C, Ar-C), 135.31 (1C, Ar-C), 133.21 (1C, Ar-C), 132.58 (1C, Ar-C), 131.15 (1C, Ar-C), 130.20 (1C, Ar-C), 128.11 (1C, Ar-C), 125.16 (1C, Ar-C), 123.49 (1C, CH), 119.07 (1C, CN), 113.11 (1C, Ar-C). DEPT-135 (125 MHz, DMSO-d_6, δ, ppm): 143.63, 135.32, 133.21, 132.59, 131.15, 130.20, 128.11, 125.15, 123.49.

(E)-4-(3-(4-nitrophenyl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch5): Color: Yellow solid. M.p.: 170-172 °C. ^{1}H NMR (500 MHz, DMSO-d_6, δ, ppm): 8.028-7.977 (t, 3H, Ar-H and α-CH), 7.941-7.924 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.887-7.870 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.640-7.609 (d, *J* = 16 Hz, 1H, β-CH), 6.645-6.628 (d, *J* = 8.5 Hz, 2H, Ar-H). ^{13}C NMR (125 MHz, DMSO-d_6, δ, ppm): 186.13 (1C, C=O), 154.49 (1C, Ar-C), 140.24 (1C, CH), 139.74 (1C, Ar-C), 133.11 (1C, Ar-C), 131.82 (1C, Ar-C), 129.53 (1C, Ar-C), 126.32 (1C, Ar-C), 125.5 (1C, CH), 119.18 (1C, CN), 113.20 (1C, Ar-C), 112.17 (1C, Ar-C). DEPT-135 (125 MHz, DMSO-d_6, δ, ppm): 139.74, 133.12, 131.82, 129.54, 126.30, 113.20.

2.3. Single-crystal XRD data collection

Single-crystal XRD analysis including data collection, cell refinement, and data reduction was performed with a Stoe IPDS2 area detector using Stoe IPDS2 software [18] and graphite-monochromated MoKα (λ = 0.71073 Å) at 100(2) K Twin integration. The structure was solved by direct methods using SIR2004 [19] and all non-hydrogen atoms were anisotropically refined by full-matrix least squares on F^2 using SHELXL [20]. Cell refinement: APEX2 and SAINT [21,22]; Data reduction: SAINT and XPREP [22,23]; Program(s) used to refine structure: SHELXL [20]; molecular graphics: ORTEP-3 [24] for Windows and Mercury [25] software used to prepare material for publication: SHELXL [20] and PLATON [26]. The integration and scaling were performed to obtain reflection profiles from each of the twin components. A component was used to determine the space group, followed by the determination of the initial structure by the direct method (SHELX) [27] using the crystallographic CRYSTALS program [28].

3. Results and discussion

3.1. Synthesis of five novel chalcone molecules (Ch1-5)

Initially, all molecules were prepared by our earlier developed KOH-catalyzed process [29,30]. Thereafter, to have a comparative investigation, we tried to prepare all five structures with the use of pyrrolidine as the catalyst while remaining all parameters. During this study, pyrrolidine was clearly observed to be an effective alternative to KOH. In both processes, we were able to obtain a greater amount of yield with pyrrolidine than KOH (Table 1). The structure of the synthesized compounds was confirmed by infrared (IR), NMR, HR-MS, UV-vis, and single-crystal XRD spectral analysis.

3.2. FT-IR and HR-MS spectroscopic studies

The vibrational stretching frequency of the aromatic chalcones was analyzed by FT-IR spectroscopy. The FTIR spectrums of all prepared chalcones have shown a characteristic absorption band at 2260-2222 cm^{-1} corresponding to the CN stretching frequency. The existence of the C=O group was confirmed by IR spectral data, which showed sharp bands in the range of 1625-1660 cm^{-1} in the presence of conjugated ketones, suggesting the presence of the described compounds. The absorption band at 1627 cm^{-1} indicates the presence of α,β-unsaturated ketone which confirms the formation of chalcone.

3.3. NMR spectroscopic studies

Spectral analysis by ^{1}H NMR and ^{13}C NMR revealed the structure of all these compounds (Ch1-5). The chalcones appeared to be geometrically pure and configured *trans* (J_{Ha-Hb} = 16 Hz) according to ^{1}H NMR spectra. The methoxy proton in Ch2 chalcone was observed at δ 3.986 ppm. In the ^{13}C NMR spectrum, carbonyl carbon was observed at δ 198 ppm and aromatic carbons were observed in the range of δ 150 to120 ppm.

Table 2. Crystal data and structure refinement for (*E*)-4-(3-(6-methoxynaphthalen-2-yl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch2).

Empirical formula	$C_{21}H_{15}NO_2$
Formula weight (g/mol)	313.34
Temperature (K)	293(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a, (Å)	6.5694(3)
b, (Å)	33.2697(15)
c, (Å)	7.4516(4)
β (°)	97.563(2)
Volume (Å^3)	1614.47(14)
Z	4
ρ_{calc} (g/cm^3)	1.289
μ (mm^{-1})	0.083
F(000)	656.0
Crystal size (mm^3)	0.3 × 0.25 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection (°)	4.898 to 49.99
Index ranges	$-7 \le h \le 7, -37 \le k \le 39, -7 \le l \le 8$
Reflections collected	16000
Independent reflections	2822 [R_{int} = 0.0249, R_{sigma} = 0.0196]
Data/restraints/parameters	2822/0/217
Goodness-of-fit on F^2	1.088
Final R indexes [I≥2σ (I)]	R_1 = 0.0484, wR_2 = 0.1141
Final R indexes [all data]	R_1 = 0.0657, wR_2 = 0.1257
Largest diff. peak/hole (e.Å^{-3})	0.17/-0.17

Table 3. Bond lengths for (*E*)-4-(3-(6-methoxynaphthalen-2-yl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch2).

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
C1	C2	1.355(3)	C11	O1	1.426(3)
C1	C6	1.409(3)	C12	C13	1.485(3)
C2	C3	1.411(3)	C12	O2	1.220(2)
C3	C4	1.361(3)	C13	C14	1.311(3)
C3	O1	1.363(2)	C14	C15	1.461(3)
C4	C5	1.412(3)	C15	C16	1.387(3)
C5	C6	1.421(3)	C15	C20	1.386(3)
C5	C10	1.412(3)	C16	C17	1.377(3)
C6	C7	1.406(3)	C17	C18	1.384(3)
C7	C8	1.371(3)	C18	C19	1.374(3)
C8	C9	1.418(3)	C18	C21	1.439(3)
C8	C12	1.479(3)	C19	C20	1.374(3)
C9	C10	1.356(3)	C21	N1	1.136(3)

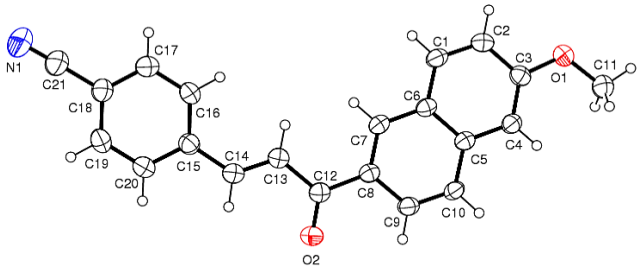


Figure 2. Molecular structure displacement ellipsoid plot drawn at 40% probability (Ch2).

Nitrile (CN) is typically observed in the range between δ 115-125 ppm deshielding due to nitrogen. The DEPT spectrum of all prepared compounds clearly confirms the presence of the corresponding quaternary carbons in the molecules.

3.4. UV-Visible spectroscopy

The π → π* transition (bathochromic shift) and the n → π* transition (hypsochromic shift) are the two main absorption maxima in chalcone derivatives [31-33]. The absorption maxima at 370 and 371 nm, respectively, in the UV-Visible spectra of chalcones Ch1 and Ch2, and the UV-Visible spectrum of the chalcone Ch3 to Ch5 and the absorption maxima at 372, 373, and 373 nm, are attributable to the π → π* transition, respectively. The productions of chalcone Ch1 to Ch5 were also confirmed by their absorption maxima seen in their respective UV spectrums.

3.5. Single-crystal XRD study

Clearly, the structure of 4-(3-(6-methoxynaphthalen-2-yl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch2) was well recognized by its single-crystal XRD studies (Figure 2). Crystal data and structure refinement for Ch2 are listed in Table 2. The H atoms were comprised in calculated positions and treated as riding atoms: C–H = 0.93–0.96 Å with Uiso(H) = 1.5 Ueq(C-methyl) and 1.2 Ueq(C) for all other H atoms in the compound [34]. The structure was refined for the molecule as a two-component twin: 180 rotations about the axis a; BASF = 0.063(1). The molecular geometry of the compound is very similar, with bond distances and angles in the expected range (Tables 3 and 4). In a single crystal structure, the polynuclear naphthalene ring and the aromatic phenyl ring with the nitrile group are almost coplanar with the α,β-unsaturated carbonyl moiety.

Table 4. Bond angles for (*E*)-4-(3-(6-methoxynaphthalen-2-yl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch2).

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
C2	C1	C6	121.19(19)	C8	C12	C13	119.26(17)
C1	C2	C3	120.44(19)	O2	C12	C8	120.68(18)
C4	C3	C2	120.08(19)	O2	C12	C13	120.05(18)
C4	C3	O1	125.59(19)	C14	C13	C12	121.62(19)
O1	C3	C2	114.33(18)	C13	C14	C15	127.7(2)
C3	C4	C5	120.63(18)	C16	C15	C14	123.05(19)
C4	C5	C6	119.22(17)	C20	C15	C14	119.26(19)
C10	C5	C4	122.88(18)	C20	C15	C16	117.7(2)
C10	C5	C6	117.89(18)	C17	C16	C15	121.4(2)
C1	C6	C5	118.39(18)	C16	C17	C18	119.8(2)
C7	C6	C1	122.41(18)	C17	C18	C21	120.8(2)
C7	C6	C5	119.19(17)	C19	C18	C17	119.5(2)
C8	C7	C6	121.96(18)	C19	C18	C21	119.7(2)
C7	C8	C9	118.35(18)	C18	C19	C20	120.3(2)
C7	C8	C12	123.01(18)	C19	C20	C15	121.3(2)
C9	C8	C12	118.62(17)	N1	C21	C18	178.4(3)
C10	C9	C8	120.97(18)	C3	O1	C11	117.73(16)
C9	C10	C5	121.61(18)				

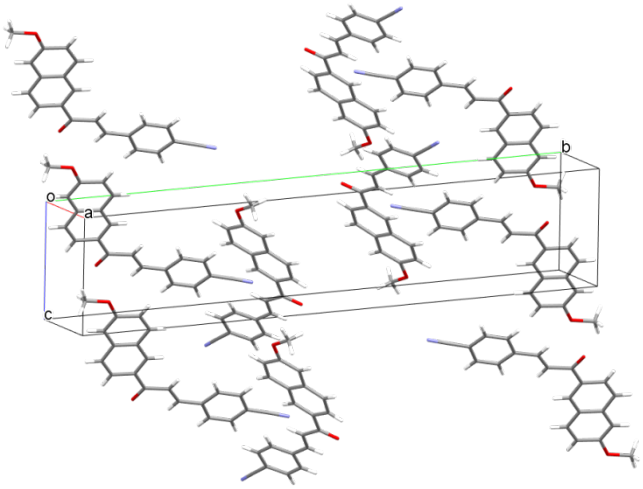


Figure 3. Unit cell diagram of (*E*)-4-(3-(6-methoxynaphthalen-2-yl)-3-oxoprop-1-en-1-yl)benzonitrile (Ch2).

In the packing structure, molecules are placed close to each other on the phenyl ring with the nitrile group, this could be due to the linear structure of the nitrile group attached to the fourth position of the phenyl ring (Figure 2). However, the naphthalene sites with the methoxy group are quite far from each other, which could be because of the nonlinear structure on the methoxy group and the bulky naphthalene ring system. As expected, the bond angles at the fusion of two rings in the naphthalene ring were significantly higher than the expected value of 120° for sp^2 hybridization. The molecule is packed with weak intermolecular C–H···O, C–H···C and C–H···N interactions using nitrile nitrogen, oxygen from methoxy and carbonyl groups. In addition, weak π-π stacking interactions are observed between naphthalene and phenyl rings. The molecular packing in the unit cell viewed from the axis *a* is presented in Figure 3.

4. Conclusions

Claisen-Schmidt condensations, catalyzed by pyrrolidine/potassium hydroxide as a base catalyst, were used to synthesize Ch1 to Ch5 derivatives. The prepared molecules were then characterized by HR-MS, FT-IR, and NMR spectroscopy. Selectively, the structure of Ch2 was established by single crystal X-ray diffraction (XRD) study. The optical properties of the chalcones were examined by using ultraviolet-visible (UV-vis) spectral data. The FT-IR spectrum of all prepared molecules shows a characteristic peak at 1660-1630 cm^{-1}, which corresponds to the C=O group of the stretching frequency, which confirms the formation of chalcones. Compounds (Ch1-Ch5) were also confirmed by ^1H NMR spectral analysis. The ^1H NMR spectra suggested that the chalcones were geometrically pure and configured *trans* (J_{Ha-Hb} = 16 Hz) to prove the formation of derivatives of the chalcones. These well-characterized structures of chalcone scaffolds with reactive functional groups (*i.e.* nitrile and 2-propenone) can be oppressed as a crucial intermediate in the synthesis of various novel heterocyclic scaffolds with numerous applications.

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Supporting information

CCDC-1431802 contains the supplementary crystallographic data for this article. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033.

Disclosure statement

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CRediT authorship contribution statement

Conceptualization: Paresh Narayan Patel; Methodology: Niteen Borane, Amar Ghanshyam Deshmukh, Nidhi Harnesh Oza; Software: Niteen Borane, Paresh Narayan Patel, Rajamouli Boddula; Validation: Paresh Narayan Patel, Rajamouli Boddula; Investigation: Paresh Narayan Patel, Rajamouli Boddula; Resources: Paresh Narayan Patel, Rajamouli Boddula; Data Curation: Paresh Narayan Patel, Rajamouli Boddula; Writing - Original Draft: Niteen Borane, Paresh Narayan Patel; Writing - Review and Editing: Niteen Borane, Paresh Narayan Patel, Rajamouli Boddula; Visualization: Paresh Narayan Patel, Rajamouli Boddula; Funding acquisition: Paresh Narayan Patel, Rajamouli Boddula; Supervision: Paresh Narayan Patel, Rajamouli Boddula; Project Administration: Paresh Narayan Patel, Rajamouli Boddula.

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