TẠP CHÍ KHOA HỌC
TRƯỜNG ĐẠI HỌC SƯ PHẠM TP HỒ CHÍ MINH
Tập 17, Số 9 (2020): 1536-1546
ISSN: 1859-3100
HO CHI MINH CITY UNIVERSITY OF EDUCATION
JOURNAL OF SCIENCE
Vol. 17, No. 9 (2020): 1536-1546
Website: *http://journal.hcmue.edu.vn*

Research Article

SYNTHESIS AND STRUCTURE OF SOME CHALCONES CONTAINING ACETAMIDE GROUP

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Received: August 03, 2020; Revised: August 18, 2020; Accepted: September 18, 2020

ABSTRACT

*Two chalcones including (E)-3-(2-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3a**) and (E)-3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3b**) were synthesized by the reaction of acetophenone and 2-hydroxybenzaldehyde or 4-hydroxybenzaldehyde, respectively. The Williamson reaction of (**3a**) or (**3b**) with the various N-aryl-2-chloroacetamides gave eight (E)-N-(4-aryl)-2-(2/4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide compounds; seven of them were new compounds: (E)-N-(4-bromophenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5a**), (E)-N-(4-chlorophenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5b**), (E)-N-(4-methoxyphenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5c**), (E)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-N-(p-tolyl)acetamide (**5d**), (E)-N-(4-bromophenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5e**), (E)-N-(4-chlorophenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5f**), (E)-N-(4-methoxyphenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5g**), (E)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-N-(p-tolyl)acetamide (**5h**). The structure of the compounds was determined by their IR, ^{1}H-NMR, ^{13}C-NMR, and HR-MS spectral data.*

Keywords: acetamide; acetophenone; chalcone; 2-hydroxybenzaldehyde; 4-hydroxybenzaldehyde

1 Introduction

Chalcone is an important intermediate biosynthetic product of shikimate pathway forming flavonoids which has many significant biological activities (Nandedkar et al., 2013). The substituted chalcones and their derivatives are reported possessing many interesting bioactivities such as antimalarial (Awasthi, Mishra, Kumar, et al., 2009; Lim et al., 2007; Motta et al., 2006), anticancer (Achanta et al., 2006; Echeverria et al., 2009; Ilango et al., 2010), anti-inflammatory (Yadav et al., 2010; Zhang et al., 2010), antimicrobial (Awasthi,

Cite this article as: Bui Thị Thuy Linh, Nguyen Tien Cong, & Huynh Thi Xuan Trang (2020). Synthesis and structure of some chalcones containing Acetamide group. *Ho Chi Minh City University of Education Journal of Science, 17*(9), 1536-1546.

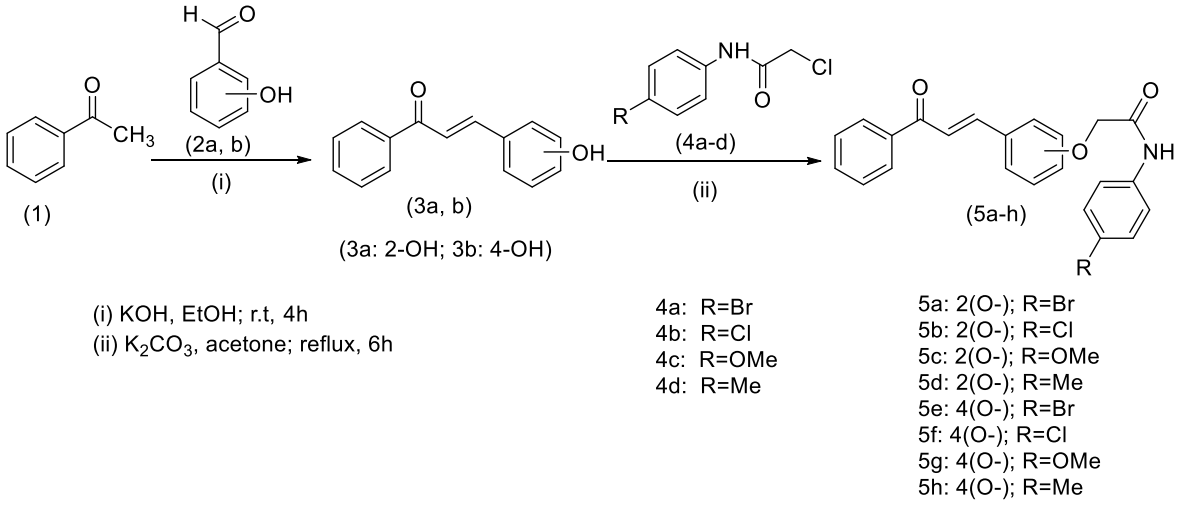
Mishra, Dixit, et al., 2009; Bag et al., 2009; Bhatia et al., 2009; Hamdi et al., 2010; Lahtchev et al., 2008) anticonvulsant (Nitin, 2010), antioxidant (Sivakumar et al., 2010; Vasil'ev et al., 2010; Vogel et al., 2008), and enzymes inhibitor (Chimenti et al., 2009; Najafian et al., 2010; Zarghi et al., 2006). Besides, chalcones are also used as a template for the synthesis of various potential therapeutic heterocyclic compounds such as pyrimidine, pyrazoline, benzofuran, thiadiazine, isoxazole, quinolinones, benzodiazepine (Abonia et al., 2008; El-Hamouly et al., 2011; Gaede & Mcdermott, 1993; Shibata et al., 1993).

On the other hand, compounds containing phenoxy-*N*-arylacetamide scaffold were reported showing many of the same potential bioactivities such as virus inhibitory including HCMV (Babkov et al., 2015), HIV-1 RT (Sankaran et al., 2011), antimicrobial (Berest et al., 2011; Nguyen et al., 2016; Rajurkar et al., 2014; Williams et al., 2015), antioxidant (Autore et al., 2010; Rajurkar et al., 2014), anticancer (Adimule et al., 2014; Rani et al., 2014), anti-inflammatory (Adimule et al., 2014; Rajurkar et al., 2014), analgesic, antipyretic (Adimule et al., 2014; Rani et al., 2015), and enzyme inhibitory (Atkinson et al., 2019; Kilic-Kurt et al., 2015; Ölgen et al., 2008; Raghavendra et al., 2012; Singh et al., 2017; Zhao et al., 2017).

As a continuous work exploring chalcones containing acetamide group (Nguyen et al., 2018), the synthesis and structure of seven new (*E*)-*N*-(4-aryl)-2-(2/4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy) acetamide compounds were reported.

2 Results and discussion

The synthetic pathway of a series of chalcones containing acetamide group (**5a-h**) is illustrated in Scheme 1.



Scheme 1. *The synthetic pathway*

Recently, compound (*E*)-3-(2-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3a**) and (*E*)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-*N*-(*p*-tolyl)acetamide (**5d**) was synthesized and spectroscopically analyzed (Nguyen et al., 2018).

The chalcones (**3a,b**) were prepared by the condensation reaction of acetophenone (**1**)

with definite 2-hydroxybenzaldehyde (**2a**) or 4-hydroxybenzaldehyde (**2b**) under alkaline condition (Anwar et al., 2018; Ngaini et al., 2009). Physical properties and IR, ^{1}H-NMR spectral data of (**3a,b**) compounds are matched with the data in a previous study (Anwar et al., 2018). In the IR spectra of the **3a** and **3b** compounds, the signal of the C=O group appeared in the low frequency around 1645 cm^{-1} due to the conjugation of the C=O and C=C bonds. Besides, absorptions corresponding to bending vibrations appeared near 970 cm^{-1} in the spectra of these compounds indicated that (**3a,b**) were *trans*-alkenes. In the ^{1}H-NMR spectra, the coupling between α-H (δ 7.73 - 7.86) and β-H (δ 7.75 - 8.08) with a *spin-spin* coupling constant (J = 16.0 – 18.0 Hz) indicated that both of chalcones (**3a,b**) exist in the (*E*)-configuration which is in agreement with IR spectral data described above.

N-aryl-2-chloroacetamides were synthesized according to the procedure described in a previous report (Nguyen et al., 2016). In this procedure, *N*-aryl-2-chloroacetamides were obtained with a high yield by acylation of corresponding substituted anilines, using chloroacetyl chloride as an acylation agent and acetic acid as a solvent.

Stirring a mixture of a definite hydroxychalcone (**3a** or **3b**) and a definite *N*-aryl-2-chloroacetamide (**4a** or **4b** or **4c** or **4d**) in acetone containing potassium carbonate gave corresponding substituted chalcones (**5a-h**). The reaction belongs to the Williamson reaction type to prepare ethers from phenols and halogen derivatives. Mass spectra of the (**5a-h**) compounds showed that the molecular peaks in agreement with their molecular formula. The IR, ^{1}H NMR, and ^{13}C-NMR spectra of the products are matched with the proposed structures. In the IR spectra of the (**5a-h**) compounds, the stretching band above 3330 cm^{-1} indicated the presence of the NH group while the strong band around 1685 cm^{-1} indicated the presence of an amide C=O group. In comparison to the ^{1}H-NMR spectra of (**3a,b**), the spectra of (**5a-h**) compounds appeared to have some extra signals in the aromatic area. Moreover, the signal of the CH_2 group as a *singlet* with the intensity of 2H at 4.77-4.90 ppm was seen easily. The ^{1}H-NMR spectra also showed the presence of vinylic protons with a coupling constant $J_{ab} \approx$ 15.5-16.0 Hz referred to *trans* conformation. However, the vinylic protons in the molecule of (**5a-d**) compounds have the characteristics of A-B systems with a slight difference in the chemical shift between signals of protons Hα and Hβ (Δδ = 0,04 ppm) while the vinylic protons in the molecule of (**5e-h**) compounds have the characteristics of A-M systems with more differences in the chemical shift between the signals of these protons (Δδ = 0,09 ppm). In addition, the electronic withdraw by the inductive effect of the oxygen atom makes the signal of the vinylic protons in (**5a-d**) compounds to appear at a lower magnetic field than those of (**5e-h**) compounds. In the ^{13}C-NMR spectra of (**5a-h**) compounds, the aliphatic carbon of the acetamide group showed a signal near 67.5 ppm.

3 Experiment

3.1 Materials and measurements

The chemicals used e.g., acetophenone (**1**), 2-hydroxybenzaldehyde (**2a**), and 4-hydroxybenzaldehyde (**2b**) were laboratory grade and supplied by Acros. Melting points were determined on a Gallenkamp apparatus and were uncorrected. Infrared (IR) spectra were recorded on a Shimadzu FTIR-8400S spectrophotometer. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance instrument (500 MHz) using deuterated dimethylsulfoxide solutions containing tetramethylsilane as an internal standard. The spin-spin coupling constants (*J*) are given in Hz. HR-MS experiments were performed using an Agilent Q-TOF 6500.

3.2 Synthesis and characterization

3.2.1 General procedure for the synthesis of chalcone (E)-3-(aryl)-1-phenylprop-2-en-1-one (3a,b)

A solution of 0.022 mol (2.64 g) acetophenone (1) was slowly added to a potassium hydroxide solution in 10 mL ethanol (3.36 g of potassium hydroxide in 15 mL ethanol) and stirred for 20-30 minutes. The solution of 2.44g (0.02 mol) hydroxybenzaldehyde respectively (**2a,b**) was continuously added dropwise to this solution. The obtained mixture was stirred for three hours at room temperature and kept overnight in a refrigerator. Then, the mixture reaction was poured into ice water and acidified with diluted HCl (1:1) until reaching pH = 3-4. The solid obtained was filtered, washed thoroughly with water, and dried. Crystallization of the crude residue from ethanol: water (4:1) afforded 68.53% (3.07 g) of (*E*)-3-(2-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3a**) as yellow solid and 42.22% (1.89 g) of (*E*)-3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3b**) as yellow cylindrical crystals.

*(E)-3-(2-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3a**)*

m.p. 148-149 °C (Ref. (Syam et al., 2012): 147-149 °C), IR (ν, cm-1, KBr): 3240 (broad, OH), 3086 (C-H), 1643 (C=O), 1600 (C=C), 967 ($\gamma_{C=C}$); ^{1}H NMR (500 MHz, DMSO-d6): δ 6.89 (1H, *dd*, $J_1 = J_2 = 7.5$, ArH), 6.96 (1H, *d*, $J = 8$, ArH), 7.29 (1H, *ddd*, $J_1 = J_2 = 8.5$, J_3=1.5, ArH), 7.57 (2H, *dd*, $J_1 = J_2$= 7.5, ArH), 7.66 (1H, *dd*, J_1 =7, J_2 = 7.5, ArH), 7.86 (1H, *dd*, J_1 = 7.5, J_2 = 1.5, ArH), 7.86 (1H, *d*, J = 16.0, α-H), 8.08 (1H, *d*, J = 17.0, β-H), 8.10 (2H, *d*, J = 7, ArH), 10.29 (1H, *s*, OH); ^{13}C NMR (125 MHz, DMSO-d6): δ 116.2, 119.4, 121.0, 121.4, 128.3, 128.7, 128.8, 132.0, 132.9, 137.9, 139.6, 157.3, 189.5.

*(E)-3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3b**)*

m.p. 198-200 °C (Ref. (Tomecková et al., 2006): 180-182 °C), IR (ν, cm-1, KBr): 3225 (broad, OH), 3017 (C-H), 1651 (C=O), 1600 (C=C), 972 ($\gamma_{C=C}$); ^{1}H NMR (500 MHz, DMSO-d6): δ 6.86 (2H, *d*, J = 8.5, ArH), 7.57 (2H, *dd*, J_1 =7.5, J_2 = 7, ArH), 7.66 (1H, *dd*, J_1=6, J_2=7, ArH), 7.73 (1H, *d*, J = 16.5, α-H), 7.75 (1H, *d*, J = 18, β-H), 7.75 (2H, *d*, J = 8, ArH), 8.13 (2H, *d*, J = 8, ArH), 10.12 (1H, *s*, OH); ^{13}C NMR (125 MHz, DMSO-d6): δ 115.8, 118.5, 125.8, 128.3, 128.7, 131.1, 132.8, 137.9, 144.5, 160.2, 189.0.

3.2.2 General procedure for synthesis of N-aryl-2-chloroacetamide compounds (4a-d)

2-Chloroacetyl chloride 3.0 g (~0.0265 mol) was added dropwise to a solution of an appropriate substituted aniline (0.025 mol) in 15 ml glacial acetic acid while being cooled in an ice-bath. After being stirred in the ice-bath for 30 minutes and then stirred for 1 hour in room temperature, the reaction mixture was poured into 50 mL cold water containing 2.05 g (0.025 mol) sodium acetate. The precipitate was filtered, then washed with cold water and recrystallized from ethanol.

N-(4-bromophenyl)-2-chloroacetamide (**4a**): white crystalline solid (4.62 g, 74.4%); mp: 174.4 ^{o}C (Ref. (Al-Sha'er, 2014): 174-176 ^{o}C);

2-chloro-*N*-(4-chlorophenyl)acetamide (**4b**): pale grayish crystalline solid (4.47 g, 87.6%); mp: 137.8 ^{o}C (Ref. (Al-Sha'er, 2014): 136-138^{o}C);

2-chloro-*N*-(4-methoxyphenyl)acetamide (**4c**): white crystalline solid (4.32 g, 86.6%); mp: 118.5 ^{o}C (Ref. (Sankaran et al., 2011): 118-120^{o}C);

2-chloro-*N*-*p*-tolylacetamide (**4d**): white crystalline solid (4.05 g, 88.3%); mp: 174.5 ^{o}C (Ref. (Sankaran et al., 2011): 174-176 ^{o}C);

3.2.3 General procedure for (E)-N-(4-aryl)-2-(2/4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (5a-h) derivatives

2.24g (0.01 mol) of definite chalcone (*E*)-3-(aryl)-1-phenylprop-2-en-1-one (**3a** or **3b**) was dissolved in 10 mL acetone, then 4.14g (0.03 mol) potassium carbonate was added, and the solution was stirred for 30 minutes. The solution of appropriate *N*-aryl chloroacetamide (0.01 mol in 10 mL acetone) was added *continuously dropwise into the mixture above.* The solution was refluxed with stirring for 6 hours and then being cooled down to room temperature. The solid $KHCO_3$ was separated out of the reaction mixture. The remaining solution was poured into cold water and stirred in 20 minutes. The separated solid was filtered, dried, and recrystallized from ethanol

(E)-N-(4-bromophenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide ***(5a)***: white needle crystals, yield 61.5 %; m.p. 196-198 °C, IR (ν, cm^{-1}, KBr): 3333 (N-H), 3046 (Csp^2–H), 2920 (Csp^3–H), 1690 (C=O), 1597 and 1546 (C=C), 1211 and 1065 (C-O-C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.90 (2H, *s*, CH_2), 7.05 (1H, *d*, *J* = 8.0, ArH), 7.09 (1H, *dd*, J_1=J_2=7.5, ArH), 7.46 (1H, *ddd*, J_1 =J_2= 8.0, J_3=1.5, ArH), 7.55 (4H, *m*, ArH), 7.66 (3H, *m*, ArH), 7.98 (1H, *dd*, J_1 = 7.5, J_2=1.5, ArH), 8.08 (1H, *d*, *J*=16.0, α-H), 8.12 (1H, *d*, *J*=16.0, β-H), 8.16 (2H, *dd*, J_1= 7.5, J_2=1.5, ArH), 10.45 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 67.5, 112.7, 115.3, 121.4, 121.4, 122.5, 123.4, 128.5, 128.8, 129.7, 131.7, 132.1, 133.1, 137.7, 137.9, 139.2, 157.1, 166.4, 189.4; HR-MS calcd for $C_{23}H_{19}BrNO_3$, 438.0548 (M+2+H); found 438.0570 $(M+2+H)^+$

(E)-N-(4-chlorophenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide ***(5b)***: white needle crystals, yield 64 %; m.p. 190-191 °C, IR (ν, cm^{-1}, KBr): 3402 (N-H), 3061 (Csp^2–H), 2914 (Csp^3–H), 1691 and 1654 (C=O), 1593, 1531 and 1487 (C=C), 1240

and 1058 (C-O-C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.90 (2H, *s*, CH_2), 7.06 (1H, *d*, *J* = 8.5, ArH), 7.09 (1H, *dd*, $J_1 = J_2 = 7.5$, ArH), 7.41 (2H, *d*, *J*=7.0, ArH), 7.46 (1H, *dd*, J_1=7.0, J_2= 7.5, ArH), 7.56 (2H, dd, J_1 =8.0, J_2= 7.5, ArH), 7.66 (1H, *dd*, J_1=J_2=7.5, ArH), 7.68 (2H, *d*, *J*=9.0, ArH), 7.97 (1H, *dd*, J_1=8.0, J_2=1.5, ArH), 8.09 (1H, *d*, *J*=16.0, α-H), 8.12 (1H, *d*, *J*=16.0, β-H), 8.17 (2H, *d*, *J* = 7, ArH), 10.41 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 68.0, 113.2, 121.5, 121.9, 123.1, 123.9, 127.7, 128.9, 129.2, 129.2, 130.2, 132.6, 133.5, 137.9, 138.2, 139.6, 157.6, 166.9, 189.9; HR-MS calcd for $C_{23}H_{18}ClNNaO_3$, 414.0873 (M+Na); found, 414.0868 $(M+Na)^+$.

(E)-N-(4-methoxyphenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide ***(5c)***: white needle crystals, yield 62.5 %; m.p. 172-173 °C, IR (ν, cm^{-1}, KBr): 3336 (N-H), 3001 (Csp^2–H), 2918 (Csp^3–H), 1681 and 1653 (C=O), 1598, 1541 and 1489 (C=C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 3.74 (3H, *s*, CH_3), 4.85 (2H, *s*, CH_2), 6.92(2H, d, J=9, ArH), 7.08 (2H, *m*, ArH), 7.46 (1H, *dd*, J_1=7.0, J_2=8.5, ArH), 7.55 (4H, *m*, ArH), 7.67 (1H, *dd*, J_1=7.0, J_2=7.5, ArH), 7.97 (1H, *d*, *J*=6.5, ArH), 8.08 (1H, *d*, *J*=16.0, α-H), 8.12 (1H, *d*, *J*=16.0, β-H), 8.17 (2H, *d*, *J*=7.5, ArH), 10.12 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 55.7, 68.1, 113.2, 114.4, 121.5, 121.8, 123.0, 123.9, 128.9, 129.2, 130.2, 132.0, 132.6, 133.5, 138.2, 139.7, 156.0, 157.7, 166.1, 189.9; HR-MS calcd for $C_{24}H_{21}NNaO_4$, 410.1368 (M+Na); found, 410.1371 $(M+Na)^+$

(E)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-N-(p-tolyl)acetamide ***(5d)***: white needle crystals, yield 59%; m.p. 200-202 °C (Ref. (Nguyen et al., 2018): 200-202 ºC), IR (ν, cm^{-1}, KBr): 3410 and 3155 (N-H), 3063 (Csp^2–H), 2924 (Csp^3–H), 1690 (C=O), 1659 and 1597 (C=C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 2.28 (3H, *s*, CH_3), 4.87 (2H, *s*, CH_2), 7.05 (1H, *d*, *J*=8.0, ArH), 7.09 (1H, *dd*, J_1=J_2=7.5, ArH), 7.15 (2H, *d*, *J*=8.5, ArH), 7.46 (1H, *ddd*, J_1=7.5, J_2=8.0, J_3=1.5, ArH), 7.54 (4H, m, ArH), 7.67 (1H, *dd*, J_1= J_2=7.5, ArH), 7.97 (1H, *dd*, J_1 = 7.5, J_2 = 1.5, ArH), 8.08 (1H, *d*, *J*=16.0, α-H), 8.12 (1H, *d*, *J*=16.0, β-H), 8.17 (2H, *dd*, J_1=8.0, J_2=1.5, ArH), 10.24 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 20.5, 67.6, 112.7, 119.5, 121.3, 122.5, 123.4, 128.5, 128.8, 129.2, 129.7, 132.1, 132.6, 133.1, 135.9, 137.7, 139.2, 157.2, 165.9, 189.4; HR-MS calcd for $C_{24}H_{21}NNaO_3$, 394.1419 (M+Na); found, 394.1446 $(M+Na)^+$.

(E)-N-(4-bromophenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide ***(5e)***: white needle crystals, yield 66 %; m.p. 173-174 °C, IR (ν, cm^{-1}, KBr): 3369 (N-H), 3057 (Csp^2–H), 2983 (Csp^3–H), 1684 and 1653 (C=O), 1589, 1531 and 1485 (C=C), 1242 and 1064 (C-O-C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.72 (2H, *s*, CH_2), 7.00 (2H, *d*, *J*=8.5, ArH), 7.43 (2H, *d*, *J*=8.5, ArH), 7.48 (2H, *dd*, J_1=7.5, J_2=8.0, J_3=1.5, ArH), 7.54 (2H, *d*, *J*=8.5, ArH), 7.58 (1H, *dd*, J_1=J_2=7.5, ArH), 7.64 (1H, *d*, *J*=15.5, α-H), 7.74 (1H, *d*, *J*=15.5, β-H), 7.79 (2H, *d*, *J*=9.0, ArH), 10.18 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 67.6, 115.6, 115.9, 120.5, 122.1, 128.5, 128.9, 129.2, 131.2, 132.1, 133.4, 138.2, 138.3, 144.3,

160.3, 166.9, 189.5; HR-MS calcd for $C_{23}H_{19}BrNO_3$, 438.0548 (M+2+H); found 438.0538 $(M+2+H)^+$.

*(E)-N-(4-chlorophenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5f**)*: white needle crystals, yield 64 %; m.p. 165-166 °C, IR (ν, cm^{-1}, KBr): 3369 (N-H), 3059 (Csp^2–H), 2914 (Csp^3–H), 1678 and 1647 (C=O), 1589, 1533 and 1489 (C=C), 1257 and 1058 (C-O-C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.81 (2H, *s*, CH_2), 7.39 (2H, *d*, *J*=8.5, ArH), 7.57 (2H, *dd*, J_1=7.5, J_2=8.0, ArH), 7.68 (3H, *m*, ArH), 7.74 (1H, *d*, *J*=16.0, α-H), 7.83 (1H, *d*, *J*=15.5, β-H), 7.89 (2H, *d*, *J*= 8.5, ArH), 8.14 (2H, *d*, *J*=7.5), 10.27 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 67.6, 115.6, 120.5, 121.8, 127.8, 128.5, 128.9, 129.1, 129.2, 131.2, 133.4, 137.8, 138.3, 144.3, 160.3, 166.9, 189.5; HR-MS calcd for $C_{23}H_{18}ClNNaO_3$, 414.0873 (M+Na); found, 414.0868 $(M+Na)^+$

*(E)-N-(4-methoxyphenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5g**)*: white needle crystals, yield 61 %; m.p. 157-158 °C, IR (ν, cm^{-1}, KBr): 3381 (N-H), 3039 (Csp^2–H), 2908 (Csp^3–H), 1680 and 1656 (C=O), 1589, 1543 and 1435 (C=C), 1242 and 1064 (C-O-C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 3.74 (3H, *s*, -CH_3), 4.77 (2H, *s*, CH_2), 6.91 (2H, *d*, *J*=9.0, ArH), 7.10 (2H, *d*, *J*=9.0, ArH), 7.54 (2H, *d*, *J*=8.0, ArH), 7.58 (2H, *dd*, *J*=7.0, ArH), 7.67 (1H, *dd*, *J*=7.0, ArH), 7.74 (1H, *d*, *J*=15.5, α-H), 7.83 (1H, *d*, *J*=15.5, β-H), 7.89 (2H, *d*, *J*=9.0, ArH), 8.15 (2H, *d*, *J*=7.5, ArH), 10.00 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 55.7, 67.6, 114.3, 115.6, 120.4, 121.8, 128.4, 128.9, 129.2, 131.2, 131.9, 133.4, 138.3, 144.3, 156.1, 160.4, 166.2, 189.5; HR-MS calcd for $C_{24}H_{22}NO_4$, 388.1549 (M+H); found, 388.1542 $(M+H)^+$.

*(E)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-N-(p-tolyl)acetamide (**5h**)*: white needle crystals, yield 56 %; m.p. 159-160 °C, IR (ν, cm^{-1}, KBr): 3377 (N-H), 3037 (Csp^2–H), 2908 (Csp^3–H), 1681 and 1656 (C=O), 1591, 1533 and 1431 (C=C), 1246 and 1064 (C-O-C); ^{1}H NMR (500 MHz, DMSO-d_6): δ 2.27 (3H, *s*, -CH_3), 4.78 (2H, *s*, CH_2), 7.10 (2H, *d*, *J*=8.5, ArH), 7.14 (2H, *d*, *J*=8.5, ArH), 7.53 (2H, *d*, *J*=8.5, ArH), 7.57 (2H, *dd*, J_1=*8*, J_2=7.5, ArH), 7.67 (1H, *dd*, J_1=7.5, J_2=7, ArH), 7.74 (1H, *d*, *J*=15.5, α-H), 7.83 (1H, *d*, *J*=15.5, β-H), 7.89 (2H, *d*, *J* = 8.5, ArH), 8.15 (2H, *d*, *J*=8.5, ArH), 10.04 (1H, *s*, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ 20.9, 67.6, 115.6, 120.2, 120.4, 128.4, 128.9, 129.2, 129.6, 131.2, 133.2, 133.4, 136.3, 138.3, 144.3, 160.4, 166.4, 189.5; HR-MS calcd for $C_{24}H_{21}NNaO_3$, 394.1419 (M+Na); found, 394.1411 $(M+Na)^+$.

4 Conclusions

Along with (*E*)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-*N*-(*p*-tolyl)acetamide, seven new (*E*)-*N*-(4-aryl)-2-(2/4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide compounds were synthesized starting from acetophenone and 2-hydroxybenzaldehyde or 4-hydroxybenzaldehyde. The structure of the compounds was elucidated by their IR, ^{1}H-NMR, ^{13}C-NMR, and HR-MS spectral data.

❖ ***Conflict of Interest:*** *Authors have no conflict of interest to declare.*

❖ ***Acknowledgments:*** *Financial support from the science technology fund of Nguyen Tat Thanh University for this work is acknowledged. The authors are highly indebted to team of collaborators from Ho Chi Minh university of Education.*

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TỔNG HỢP VÀ CẤU TRÚC CỦA MỘT SỐ CHALCONE CHỨA NHÓM ACETAMIDE

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Ngày nhận bài: 03-8-2020; ngày nhận bài sửa: 18-8-2020, ngày chấp nhận đăng: 18-9-2020

TÓM TẮT

*Hai chalcone là (E)-3-(2-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3a**) và (E)-3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one (**3b**) đã được tổng hợp tương ứng từ phản ứng của acetophenone với 2-hydroxybenzaldehyde hoặc 4-hydroxybenzaldehyde. Phản ứng Williamson giữa (**3a**) hoặc (**3b**) với các N-aryl-2-chloroacetamide khác nhau đã tạo thành 8 hợp chất (E)-N-(4-aryl)-2-(2/4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide; 7 trong số đó là chất mới: (E)-N-(4-bromophenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5a**), (E)-N-(4-chlorophenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5b**), (E)-N-(4-methoxyphenyl)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5c**), (E)-2-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-N-(p-tolyl)acetamide (**5d**), (E)-N-(4-bromophenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5e**), (E)-N-(4-chlorophenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5f**), (E)-N-(4-methoxyphenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)acetamide (**5g**), (E)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenoxy)-N-(p-tolyl)acetamide (**5h**). Cấu trúc của các hợp chất đã được xác nhận qua các phổ IR, ^{1}H-NMR, ^{13}C-NMR và phổ HR-MS.*

Từ khóa: acetamide; acetophenone; chalcone; 2-hydroxybenzaldehyde; 4-hydroxybenzaldehyde