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Synthesis, Characterization and Biological Evaluation of Pyrazole and their Application

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Abstract

We synthesised novel pyrazole derivatives namely, 3-(4-(4-(4-methoxyphenoxy) phenoxy) phenyl)-5-substituted phenyl-1H-pyrazole(5a-f) synthesised from 1-(4-(4-(4-methoxy phenoxy) phenoxy)phenyl)-3-substituted phenylprop-2-en-1-one (4a-f) and hydrazine hydrate. The Chalcone,1-(4-(4-methoxy phenoxy) phenyl)-3-substituted phenylprop-2-en-1-one (4a-f) were synthesised from substituted aromatic aldehydes (a-f) and 1-(4-(4-(4-methoxy phenoxy) phenoxy)phenyl)ethanone (3). The 1-(4-(4-(4-methoxy phenoxy) phenoxy) phenyl) ethanone (3) was synthesised from 1-chloro-4-(4-methoxyphenoxy)benzene (1) and 1-(4- hydroxy phenyl)ethanone (2). All synthesized compounds were characterized by using elemental and spectroscopic analysis. Antimicrobial studies of all synthesized compounds were tested against gram +ve and gram –ve bacteria.

Keywords: pyrazoles, Chalcones, Antimicrobial activity, Spectroscopic analysis.

Introduction

The nitrogen containing heterocyclic compounds are shows various biological and pharmaceutical activitie[1-3]. One of the nitrogen containing heterocyclic compounds says, pyrazole shows activities like, anti-inflammatory, Anti-cancer Activity, Anti-diabetic Activity, Anti-tubercular Activity, Analgesic Activity and Antimicrobial Activity[4-12].By reviewing the literatera of pyrazole and in connection of our earlier work[13,14] here I submit a research about the synthesizing novel novel pyrazole derivatives namely, 3-(4-(4-(4-methoxy phenoxy) phenoxy)phenyl)-5-substituted phenyl-1H-pyrazole(5a-f) from chalcones. The reaction scheme shown in Figure-1.

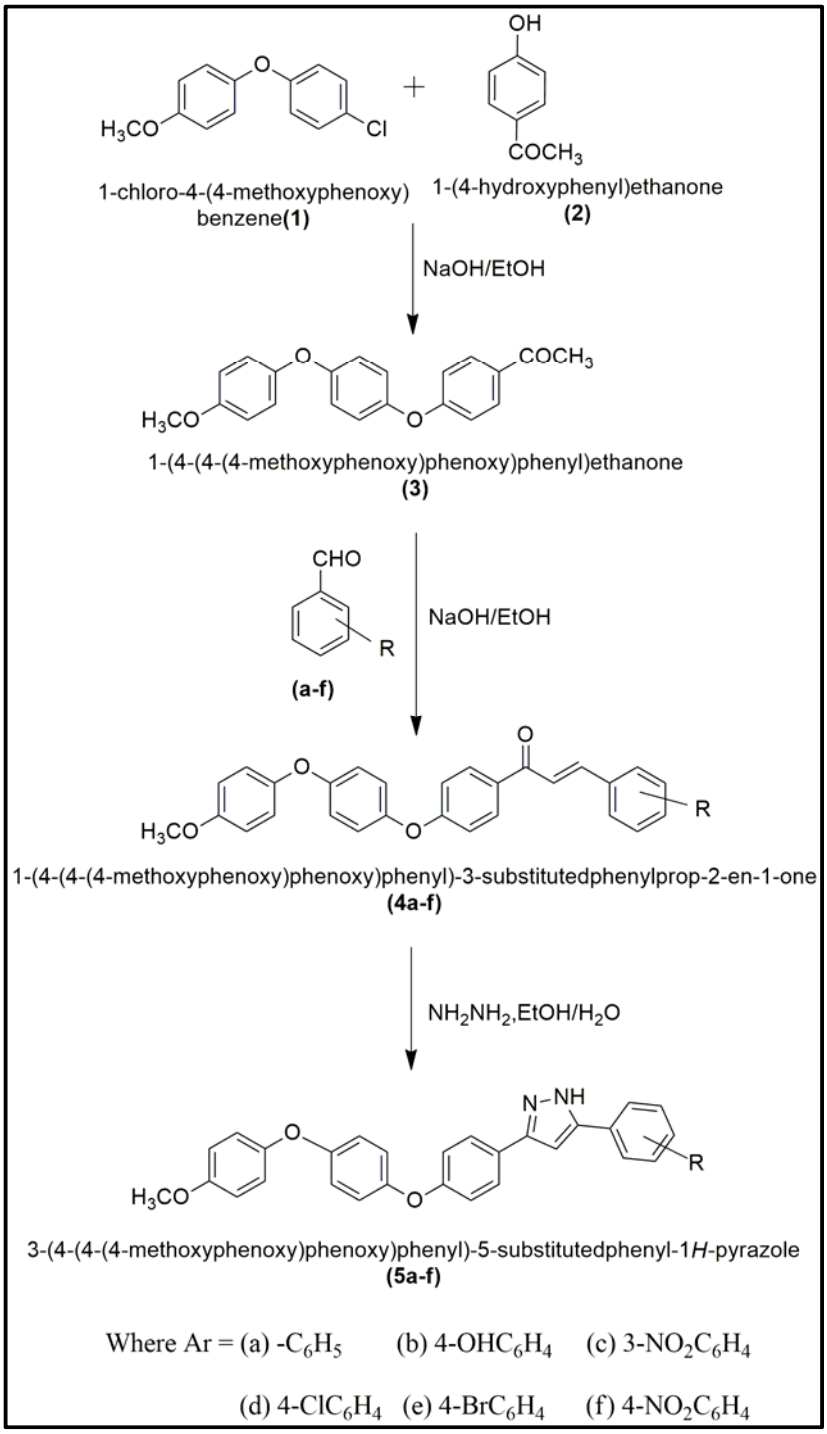


Figure-1 Reaction scheme

EXPERIMENTAL

Materials and Methods

All chemicals utilized were of laboratory reagent grade and were used as received without additional purification. Melting points were determined uncorrected using Gallenkamp melting point equipment. Carbon-Hydrogen-Nitrogen (CHN) analyzer used for elemental analyses. IR and NMR spectra done by Pye-Unicam SP-3-300 IR spectrophotometer (KBr Dicks) and Varian Mercury VX-300 and BrukerAvance III NMR spectrometer utilized DMSO-d6 as an internal standard. Mass spectra carried out using a Shimadzu GCMS-QP-1000EX mass spectrometer. The Antimicrobial Activity of all synthesized compounds was carried out by disc plate process[15].

Synthesis of 1-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)ethanone (3)

In a 250 ml round bottom flask, dissolved 1-chloro-4-(4-methoxyphenoxy)benzene (1) (0.01mol) and 1-(4-hydroxyphenyl)ethanone (2) (0.01 mol) in 30ml ethanol, add 40ml 10% NaOH with constant stirring maintaining the temperature below 25°C. After the completion of dissolution, the mixture was refluxed for 2 hr[16,17]. Then it was cooled and poured into crushed ice. Solid was separated by filtration and crystalline from ethanol. Yield, 87%, m.p. 59-60°C. It was characterized by elemental and spectral study.

Synthesis of 1-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)-3-substituted phenylprop-2-en-1-one (4a-f)

To a well stirred solution of 1-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)ethanone (3) (0.01 mol) in ethanol (30 ml) and 40% sodium hydroxide (40 ml), substituted aromatic aldehydes (a-f) (0.01 mol) was added drop wise at 0°C. After the completion of addition, the mixture was stirred for further 2-3 hr. The contents were poured into ice water and crystallized from ethanol to produced Chalcones,1-(4-(4-methoxyphenoxy)phenyl)-3-substituted phenylprop-2-en-1-one (4a-f)[16,17]. It was characterized by elemental and spectral study. The yield, M.P. and Elemental analysis are shown in Table-1.

Table-1: Analysis of compounds (4a-f)

Comp. No.	Molecular Formula	M.P.* ˚C	% Yiled	Elemental Analysis			
				C%	H%	N%	X%
				Calcd. (Found)	Calcd. (Found)	Calcd. (Found)	Calcd. (Found)
4a	$C_{28}H_{22}O_4$ (422 gm/mol)	103-104	85	79.60 79.5	5.25 5.2	-	-
4b	$C_{28}H_{22}O_5$ (438 gm/mol)	107-108	79	76.70 76.6	5.06 5.0	-	-
4c	$C_{28}H_{21}NO_6$ (467 gm/mol)	117-118	83	71.94 71.9	4.53 4.5	3.00 2.9	-
4d	$C_{28}H_{21}O_4Cl$ (456.5 gm/mol)	122-123	82	73.60 73.5	4.63 4.6	-	7.76 7.7

4e	$C_{28}H_{21}O_4Br$ (500 gm/mol)	115-116	81	67.08 67.0	4.22 4.2	-	15.94 15.9
4f	$C_{28}H_{21}NO_6$ (467 gm/mol)	122-123	84	71.94 71.9	4.53 4.5	3.00 2.9	-

***** Uncorrected. LC-MS data for 4e:500.7

Synthesis of 3-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)-5-substitutedphenyl-1H-pyrazole (5a-f)

Chalcones, 1-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)-3-substituted phenylprop-2-en-1-one (4a-f) (0.01 mol) were reflux with hydrazine hydrate (0.01 mol) in the presence of NaOH under ethanol as the solvent to produced pyrazole, 3-(4-(4-methoxy phenoxy) phenyl)-5-substituted phenyl-1H-pyrazole (5a-f) within time period of 25-40 min. Then it was cooled and poured into crushed ice. Solid was separated by filtration and crystalline from ethanol[16,17]. It was characterized by elemental and spectral study. The yield, M.P. and Elemental analysis are shown in Table-2.

Table-2: Analysis of compounds (5a-f)

Comp. No.	Molecular Formula	M.P.* ˚C	% Yiled	Elemental Analysis			
				C%	H%	N%	X%
				Calcd. (Found)	Calcd. (Found)	Calcd. (Found)	Calcd. (Found)
5a	$C_{28}H_{22}N_2O_3$ (434 gm/mol)	267-268	75	77.40 77.3	5.10 5.0	6.45 6.4	-
5b	$C_{28}H_{22}N_2O_4$ (450 gm/mol)	255-256	70	74.65 74.6	4.92 4.9	6.22 6.2	-
5c	$C_{28}H_{21}N_3O_5$ (479 gm/mol)	244-45	80	70.14 70.1	4.41 4.4	8.76 8.7	-
5d	$C_{28}H_{21}N_2O_3Cl$ (468.5 gm/mol)	247-248	78	71.72 71.7	4.51 4.5	5.97 5.9	7.56 7.5
5e	$C_{28}H_{21}N_2O_3Br$ (512 gm/mol)	232-233	79	65.51 65.5	4.12 4.1	5.46 5.4	15.56 15.5
5f	$C_{28}H_{21}N_3O_5$ (479 gm/mol)	239-240	81	70.14 70.1	4.41 4.4	8.76 8.7	-

***** Uncorrected. LC-MS data for 5e:512.9

RESULTS AND DISCUSSION

The 1-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)ethanone (3) was synthesised from 1-chloro-4-(4-methoxyphenoxy)benzene (1) and 1-(4-hydroxyphenyl)ethanone (2) The elemental analysis of (3) has mol. formula: $C_{21}H_{18}O_4$ (334 gm/mole) : %C, 75.43, %H, 5.43; found : %C, 75.4, %H, 5.4; The spectral analysis of (3) are as- IR(υ,cm^{-1}): 3050-3000 (C–H aromatic st.), 2882 (CH, str, aliphatic),1686 (C=O), 1240-1220(C-O-), 1485, 1472 (C=C, str. ring), 750(C-H

def, aromatic);1HNMR (400 MHz, CDCl3,δ,ppm): 2.52(s, 3H, -CH_3),3.85 (s, 3H, -OCH_3), 6.90-8.00 (m, 8H, Ar-H); 13C NMR(100 MHz, CDCl3,δ,ppm): 26.8,197.2,130.0,128.7,117.6,161.6, 149.5,120.1,114.2,154.0, 56.1. and M^+ peak at 334.8(m/z).

The 1-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)ethanone (3) was reacted with substituted aromatic aldehydes (a-f) yielded 1-(4-(4-methoxyphenoxy)phenyl)-3-substituted phenylprop-2-en-1-one (4a-f). The yield, M.P. and Elemental analysis are shown in Table-1. The specteral study of (4a-f) are seen IR(υ,cm^{-1}): 3050-3000 (C–H aromatic st.), 2880 (CH, str, aliphatic),1660-1650 (C=O), 1260,1050(C-O-), 1660-1570 (C=C, str. ring), 750(C-H def, aromatic);1HNMR (400 MHz,CDCl3,δ,ppm):7.20-7.50(d, 2H, -CH=CH),3.87 (s, 3H, -OCH_3), 6.85-8.20 (m, 8H, Ar-H), (a) 6.70-7.60(m,5H,Ar-H), (b) 5.37(s,1H,-OH),6.70-7.60(m,4H,Ar-H), (c) 7.70-8.35(m,4H,Ar-H) ,(d) 7.50-7.70(m,4H,Ar-H), (e) 7.60-7.65(m,4H,Ar-H), (f) 8.05 -8.25(m,4H,Ar-H); 13C NMR(100 MHz, CDCl3,δ,ppm): 128.7, 128.2, 135.4, 145.3, 121.5, 189.9, 131.2, 129.8, 118.2, 163.0,149.5, 120.0, 114.2, 153.9,56.1.

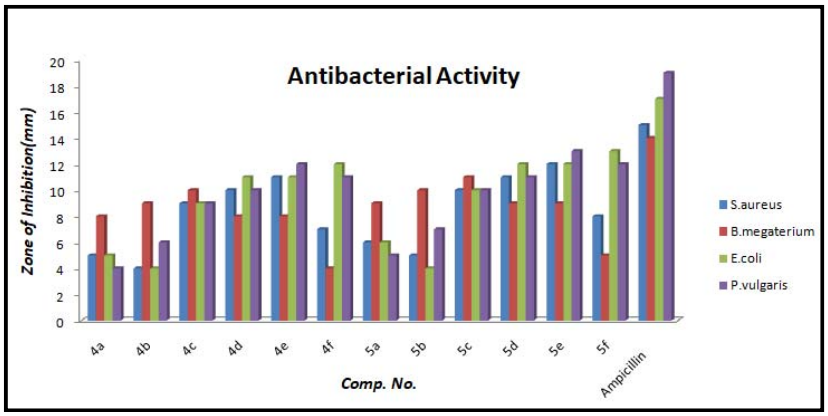
This Chalcones, 1-(4-(4-(4-methoxy phenoxy) phenoxy) phenyl)-3-substituted phenyl prop-2-en-1-one (4a-f) were reflux with hydrazine hydrate to synthesised 3-(4-(4-methoxy phenoxy)phenyl)-5-substituted phenyl-1H-pyrazole(5a-f). It shows IR(υ,cm^{-1}): 3545 (N-H st.), 3050-3000 (C–H aromatic st.), 2935,2810 (CH, str, aliphatic),1660-1650 (C=O), 1595-1569, 1115-1110(C-O-), 1650-1610 (C=C str.), 742-750(C-H def, aromatic); 1HNMR (400 MHz, CDCl3, δ,ppm):3.60 (s, 3H,-OCH_3),4.52(s,1H,-CH of Pyrazole ring), 5.60 (s, 1H, -NH), 6.85-8.20 (m, 8H, Ar-H), (a) 6.70-7.60 (m,5H,Ar-H), (b) 5.37(s,1H,-OH), 6.70-7.60 (m, 4H, Ar-H), (c) 7.70-8.35(m,4H,Ar-H) ,(d) 7.50-7.70 (m, 4H, Ar-H), (e) 7.60 -7.65 (m, 4H, Ar-H),(f)8.05-8.25(m,4H,Ar-H);13C NMR (100MHz, CDCl3,δ,ppm):129.4,128.9,127.7,133.2,99.9,147.9,126.3,127.4,118.2,157.2, 157.2,149.5,120.0, 114.2, 153.9, 56.2.

All the elemental and spectral features suggest that the data are consistent with the predicted structure shown in Scheme-1. The LC-MS of selected compounds shows the peak of M^+ ion which is consistent of their molecular weight. All these facts confirm the structures **(4a-f)** and **(5a-f)**.

Table-3: Antibacterial Activity of Compounds (4a-f) and (5a-f)

Comp. No.	***Zone of Inhibition(mm)***			
	Gram +ve		***Gram -ve***	
	S.aureus	***B.megaterium***	***E.coli***	***P.vulgaris***
4a	5	8	5	4
4b	4	9	4	6
4c	9	10	9	9
4d	10	8	11	10
4e	11	8	11	12
4f	7	4	12	11
5a	6	9	6	5
5b	5	10	4	7

5c	10	**11**	10	10
5d	11	9	12	11
5e	**12**	9	12	**13**
5f	8	5	**13**	12
Ampicillin	15	14	17	19



The examination of antibacterial activities data reveals that all compounds toxic against microbes and the compounds 5e found more active against *S.aureus and P.vulgaris,5c* found more active against *B.megaterium and 5f* found more active against *E.coli*.

CONCLUSION

The novel pyrazole derivatives namely, 3-(4-(4-(4-methoxyphenoxy)phenoxy)phenyl)-5-substituted phenyl-1H-pyrazole(5a-f) synthesised from 1-(4-(4-(4-methoxy phenoxy) phenoxy) phenyl)-3-substitutedphenylprop-2-en-1-one (4a-f) and hydrazine hydrate, which shows elemental and spectral data are consistent with predicted structure shown in reaction scheme-1.The novel synthesised compounds shows moderate to good antibacterial activities against selected pathogens.

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

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