International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064
Index Copernicus Value (2015): 78.96 | Impact Factor (2015): 6.391

Synthesis and Characterization of Five Member Ring Heterocyclic Derivatives Compounds

Mohammed R. Ahamad[1], Taghreed S. Hussain[2]

[1]Department of Chemistry, College of Science, Baghdad University, Baghdad, Iraq
[2]Department of Chemistry, College of Science, Baghdad University, Baghdad, Iraq

Abstract: ***The present work included synthesis of some new Schiff bases derivatives of hydrazine hydrate coupled with ethyl 2-(furfurylthio)acetate this role reacted with mercapto-acetic acid,amino acetic acid, chloro acetic acid and sodium azide to synthesis five member ring heterocyclic compounds derivatives.Yields of all synthesized compounds were good. All compounds were confirmed by their melting point, FT-IR spectra , 1H-NMR spectra for some of them and C.H.N.S analysis for some ofthem.***

Keyword: Schiff bases, mercapto-acetic acid, amino acetic acid, chloro acetic acid, sodium azide

1. Introduction

Heterocyclic compounds are considered one of an important type of organic compounds due to their application in drugs and industrial studies. A variety of atoms, such as N,O,S can be incorporated into the ring structures [1]. Heterocyclic compounds are also finding an increasing used as inorganicsynthesis [2]. Furfurylmercaptan (FM) is a volatile liquid with a coffee. FM occurs naturally in coffee and is odour which, at low concentrations, resembles roasted used as a constituent of flavourings, particularly for use in chocolate, fruit, nuts and coffee [3]. The Schiff's base family is composed of natural products with critical pharmacyophores [4]. It can be used as ideal lead structures to develop agrochemicals and medicines, including fungicide [5] antimicrobialdrug. [6] anti- virals, [7] antiproliferative [8] antioxidants, [9] antibacterial [10]. 4-thiazolidinones, are five member ring heterocyclic compounds [11] contain sulfur and nitrogen atoms these compounds are not aromatic. 4-thiazolidinones have been shown to have various important biological activities such as antibacterial, antifungal, antiviral, diuretic, antituberculostatic, anti-HIV, antihistaminic, anticancer, anticonvulsant, antiinflammatory [12-16]. Oxazolidinonesare a new group of antibiotics. These synthetic drugs are active against a large spectrum of Gram-positive bacteria, including methicillin- and vancomycin-resistant staphylococci, vancomycin- resistant enterococci, penicillin-resistant pneumococci andanaerobes [17]. Imidazolinone their use as anti-Parkinsonian [18] anticonvulsant [19] and monoamine oxidase inhibitoryagents. Some noveldisubstitutedimidazolinones were investigated as anticonvulsant, and succinate dehydrogenase inhibitory agents [20]. Triazoles are five member hetero cyciliccompounds ,triazole derivatives have a broad diversity of activities, high-quality pharmacokinetic,low toxicity [21], used as corrosion inhibitors and pharmacologicalactivities [22].

2. Experimental

(2- 1)-synthesis of ethyl 2- (furfurylthiol)acetate (a). [23]
A mixture of thio furfural (3,5ml, 0.035mol),dimethylformamide (DMF) (30 ml)and triethyl amine (4ml,0.028mol) stirring at room temperature for (10 mint). Ethyl chloroacetete (3ml,0.028) was added drop wise and the reaction mixture was stirred for 1/2 h. then,it was heated at (70-80) C^0 For (8 h). The reaction mixture was poured into ice water. The oil product was separate by separating funnel off, washed with sodium bicarbonate (5%) then with water,the obtained product was recrystallized from ethanol.

(2- 2)-synthesis of 2- (furfurylthiol) acetohydrazide (b). [24]
Compound (a) (1g,0.005mol) was dissolved in absolute ethanol (20ml) and hydrazine hydrate (99%,2ml,0.063mol) was added to the mixture with stirring. Then reaction mixture was stirring for (8 h.) at room temprture .The resulting solution was pourd in petri dish,the resulting product was recrystallized from ethanol.

(2-3)-synthesis of new Schiff bases from 2- (furfuryl thiol) acetohydrazide (1-5). [25]
A mixture of compound (b) (0.008 mol) and different aromatic aldehydes (0.008 mol) in absolute ethanol (20ml) and (4-5 drops) of glacial acetic acid was refluxed in water bath for about (6 h.). The excess solvent was Concentrated Under reduced pressure .The crude product was dried, recrystallized from ethanol . Physical properties of compounds (1-5) are listed in Table (3-1).

(2-4)-synthesis of 4-thiazolidinone derivatives (6-10). [26]
A mixture of Schiff bases [1-5] (0.001mol) and excess of thioglycolic acid (0.002mol) in ethanol .The reaction was refluxed for (18-20h.).The solvent was evaporated and residue was neutralized with 5% sodium bicarbonate solution to remove excess of thioglycolic acid. The formed precipitate was filtered ,washed several time with water and recrystallized from acetone. Physical properties of compounds (6-10) are listed in Table (3-1).

(2-5)- synthesis of 1,3-oxazolidin -5-one derivatives (11-15). [27]
A solution of Schiff base (1-5) (0.001mol) in THF (20ml.) was added to a well-stirred mixture of monochloroacetic acid (0.001 mol) and using small drops of triethyl amine as catalyst. The mixture was refluxed for (15 h.) ,poured in petri dish the solid product was collected and recrystallization from ethanol solvent.Physical properties of compounds (11-15) are listed in Table (3-1).

(2-6) - synthesis of 4- imidazolinone derivatives (16-20). [28]

A mixture of Schiff bases (1-5) (0.001), α- glycine (amino acetic acid) (0.001) in ethanol (20 ml) and 5 drops of DMF. The mixture was refluxed for (20 h.),the solvent was evaporated and dried ,the solid product was collected and recrystallization from ethanol solvent . Physical properties of compounds (16-20) are listed in Table (3-1).

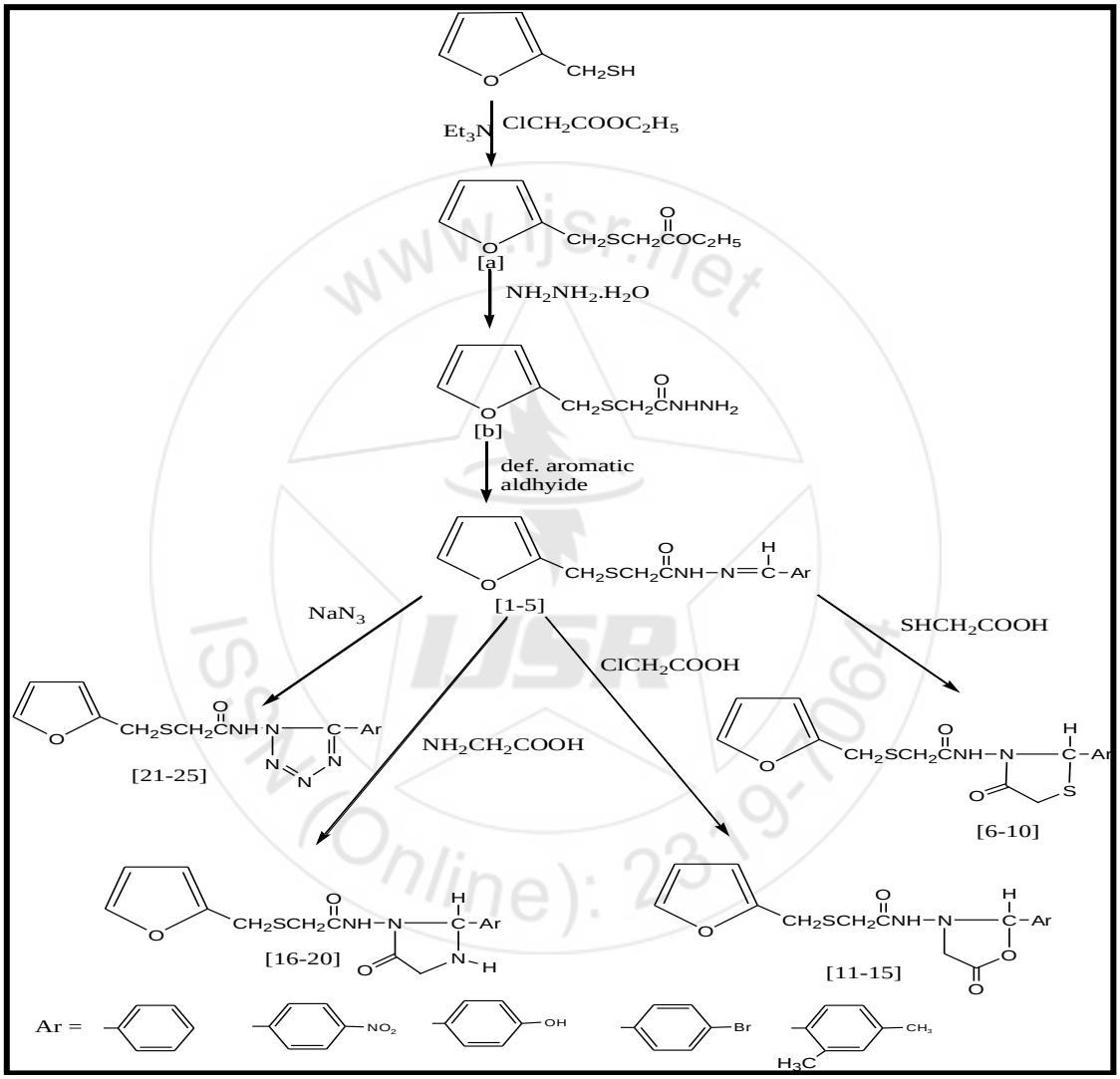
(2-7)- Synthesis of tetrazol derivatives (21-25). [29]

A mixture of Schiff base (1-5) (0.001mol) and sodium azide (0.001) in the (20ml) ethanol and 5drops of DMF. The reaction was refluxed for (20h.),the solvent was evaporated . The formed precipitate was dried, washed with water several times and recrystallized from ethanol . Physical properties of compounds (21-25) are listed in Table (3-1).

3. Results and Discussion

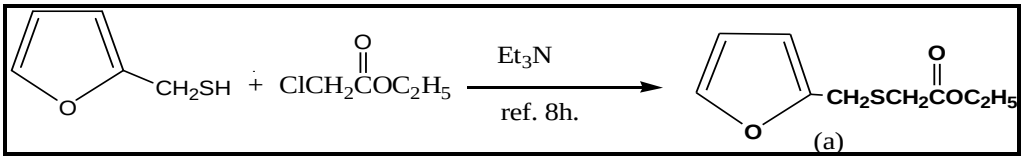
This work includes synthesis of new heterocyclic ring derivatives as shown in scheme (3-1).

Scheme (3-1)



(3-1)- ethyl 2- (furfurylthiol)acetate (a).

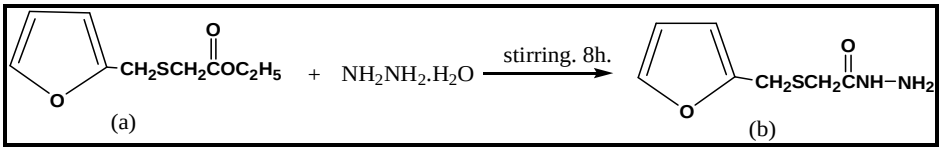
furfuryl mercaptan reacted with ethyl chloro acetate in alkali medium to prepare the compound (a) as shown in Equation (3-1). Black,B.P (219) C^0, Yield58 (%). FT-IR spectral data of compound (a) showed the appearance of characteristic absorption bands at (2979,2929) cm^{-1}belong to v (CH_3) asym. and sym. , characteristic absorption band at (1733) belong to v (C=O) cm^{-1} and disappearance of the absorption band (2567)cm^{-1} to v (S-H). 1HNMR see in Table (3-3) and figure 1. C.H.N.Sanalysis seein Table (3-4).



Equation (3-1)

(3-2)- 2- (furfuryl thiol) acetohydrazide (b).

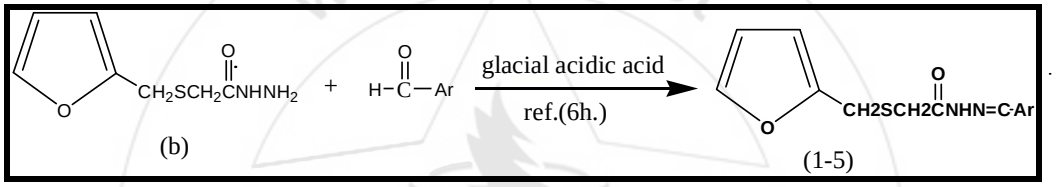
Compound (a) was treated with hydrazine hydrate in absolute ethanol with stirring at room temperature as indicated in Equatio ((3-2) to gave compound (b). Deep yellow.B.p (94) C^0 Yield 87 **(%)**. FT-IR spectra data of compound (b) showed the appearance of the characteristic absorption band at (3217-3120) cm-1belong to v (NH_2) asym. sym., characteristic absorption band at (1664)cm^{-1} v (C=O) due to amid carbonyl group and disappearance of the absorption band (1733)cm^{-1} v (C=O)due to ester carbonyl group. 1HNMR see in Table (3-3) and figure 2 .C.H.N.S analysis see in Table (3-4).



Equation (3-2)

(3-3)- new Schiff bases from 2- (furfuryl thiol) acetohydrazide (1-5).

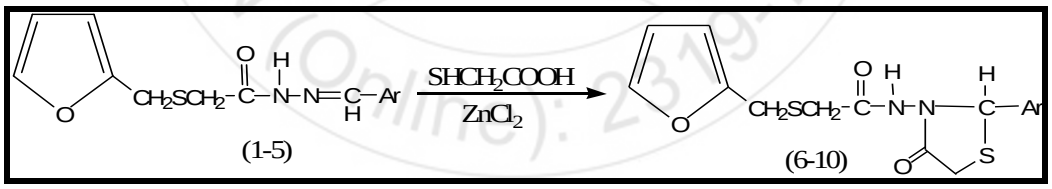
The titled compounds were synthesized from the reaction between compound (b) and appropriate aldehydes in absolute ethanol and glacial acetic acid as shown in Equation (3-3). Physical properties of the compounds (1-5) are listed in Table (3-1).FT-IR spectrum data of compounds (1-5) showed appearance of characteristic absorption bands at (3047-3180) cm^{-1} belong to v (N-H) ,characteristic absorption band at (1658-1672)cm^{-1} v (C=O)due to carbonyl of amid group, (1602-1627)cm^{-1} belong to (C=N) and disappearance of the absorption bands (3217,3120)cm-1 belong to v (NH2) asym.,sym. All details of FTIR spectral data of compounds (1-5) are listed in Table (3-2). ^{1}HNMR see in Table (3.3) and figure 3,4. C.H.N.S analysis showed in Table (3.4).



Equation (3-3)

(3- 4)- 4- thiazolidinone derivatives (6-10).

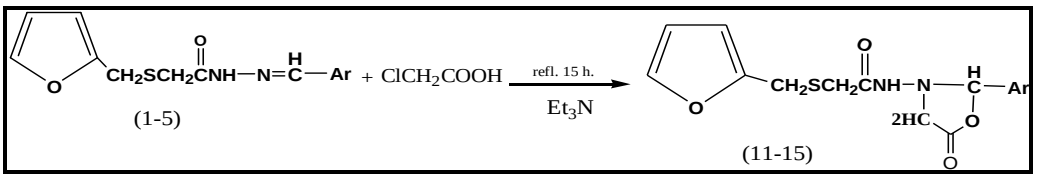
The 4- thiazolidinon derivatives (6-10) were synthesized by refluxing equimolar amounts from the compounds (1-5) with mercapto-acetic acid in ethanol as shown in Equation (3-4). Physical properties of compounds (6-10) are listed in Table (3-1). FTIR spectrum data of compounds (6-10) showed appearance of stretching band of carbonyl group at (16251674)and stretching band of carbonyl group at [1683-1733]due to thiazolidinone ring and disappearance of the absorption bands (1602-1627)cm^{-1} belong to v (C=N). All details of FTIR spectral data of compounds (6-10) are listed in Table (3-2). ^{1}HNMR see in Table (3.3) and figure 5,6. C.H.N.S analysis showed in Table (3.4).



Equation (3-4)

(3-5)- 1,3-oxazolidin -5-one derivatives (11-15).

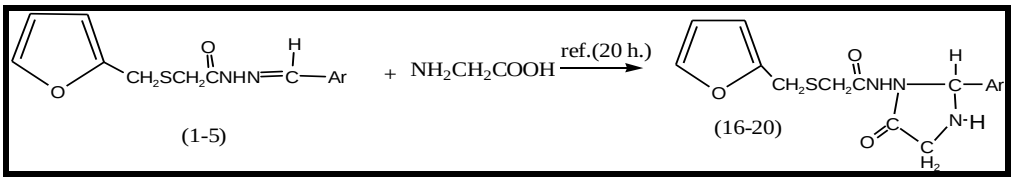
Oxazolidinone derivatives prepared by the heating of Schiff base derivatives with mono chloro acetic acid this and Et_3N as show in equation (3-5).Physical properties of the compounds (11-15) are listed in Table (3-1) . FTIR spectrum data of compounds (11-15) showed appearance of stretching band of carbonyl group at (1658-1674). and stretching band of carbonyl group at (1716-1768) due to oxazolidinone ring and disappearance of the absorption bands (1602-1627)cm^{-1} belong to v (C=N).. All details of FTIR spectral data of compounds (11-15) are listed in Table (3-2). ^{1}HNMR see in Table (3.3) and figure 7,8 .C.H.N.S analysis showed in Table (3.4).



Equation (3-5)

(3-6)- imidazolinone derivatives (16-20)

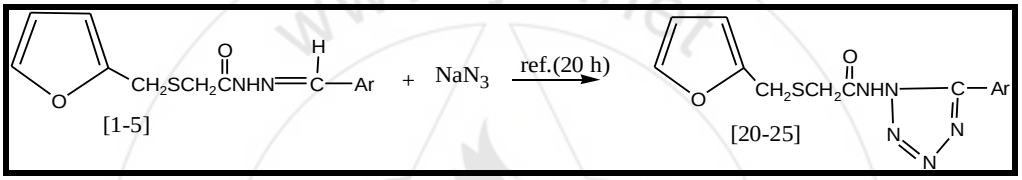
4-imidazolinone derivatives prepared by the heating of Schiff base derivatives with amino acetic acid this shows in equation (3-6). Physical properties of compounds (16-20) are listed in Table (3-1).The FTIR spectrum data of compounds (16-20) showed the appearance of stretching band of carbonyl group at (1662-1674) and stretching band of carbonyl group at (1689-1733) due to imidazolinone ring and disappearance of the C=N group in (1602-1627) for Schiff base. All details of FTIR spectral data of compounds (16-20) are listed in Table (3-2). ^{1}HNMR see in Table (3.3) and figure 9,10 . C.H.N.S analysis showed in Table (3.4).



Equation (3-6)

(3-7)- tetrazol derivatives (20-25).

Tetrazol derivatives (21-25) were synthesized py refluxing equimolar amounts from the compounds (1-5) with sodium azide as shown in Equation (3-7). Physical properties of the compounds (21-25) are listed in Table (3-1). FTIR spectrum data of compounds (21-25) showed appearance of stretching band of carbonyl group at (1662-1676). and stretching band of (N=N)at (1404-1490) for tetrazol ring. All details of FTIR spectral data of compounds (20-25) are listed in Table (3-2). ^{1}HNMR see in Table (3.3) and figure 11,12 . C.H.N.S analysis showed in Table (3.4).



Equation (3-7)

Table (3-1): Physical properties of compounds (1-25)

NO.	Formula	M.wt g/mol	(M.p.)C°	Color	Yield (%)
1	$C_{14}H_{13}O_4SN_2$	319	120-122	Brown	45
2	$C_{14}H_{14}O_3N_2S$	290	131-133	Yellow	58
3	$C_{14}H_{13}O_2N_2SBr$	352	220 D	Dark yellow	53
4	$C_{14}H_{14}O_2N_2S$	274	Oil	Light brown	87
5	$C_{16}H_{18}O_4N_2S$	334	108-110	Yellow	96
6	$C_{16}H_{15}O_5N_3S_2$	392	Decom.200	Light yellow	41
7	$C_{16}H_{16}O_4N_2S_2$	364	Decom.200	Light orange	66
8	$C_{16}H_{16}O_3N_2S_2Br$	426	186-188	Yellow	75
9	$C_{16}H_{16}O_3N_2S_2$	348	220-222	Off white	72
10	$C_{16}H_{18}O_4N_2S_2$	408	140-142	Yellow	60
11	$C_{16}H_{15}O_6N_3S$	377	120-123	Green light	56
12	$C_{16}H_{16}O_5N_2S$	348	92-94	Pale yellow	76
13	$C_{16}H_{15}O_4N_2SBr$	411	Oil	Red	60
14	$C_{16}H_{16}O_4N_2S$	332	96-98	Deep brown	50
15	$C_{18}H_{20}O_6N_2S$	392	112-116	Deep yellow	69
16	$C_{16}H_{15}O_4N_4S$	375	200-202	Yellow	52
17	$C_{16}H_{16}O_4N_3S$	346	168-170	Yellow	56
18	$C_{16}H_{15}O_3N_3SBr$	408	170-172	Orange	73
19	$C_{16}H_{16}O_3N_3S$	330	Oil	Brown	70
20	$C_{18}H_{20}O_5N_3S$	390	118-120	Brown	56
21	$C_{14}H_{12}O_4N_6S$	385	120-122	Light yellow	72
22	$C_{14}H_{13}O_3N_5S$	329	182-183	Yellow	59
23	$C_{14}H_{12}O_2N_5SBr$	391	166-168	Yellow	70
24	$C_{14}H_{12}O_2N_5S$	315	Oil	Brown	56
25	$C_{16}H_{17}O_4N_5S$	341	150-152	Off white	66

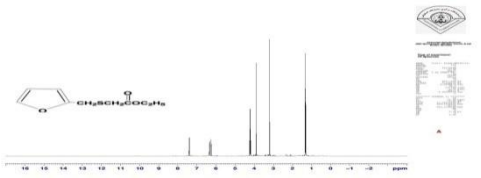


Figure 1:1HNMR Spectral of compound (a)

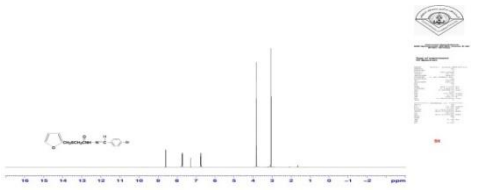


Figure 2:1HNMR Spectral of compound (b)

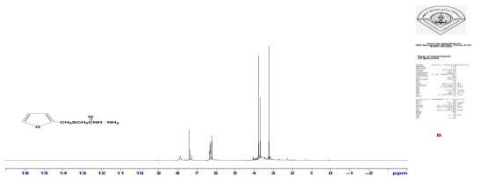


Figure 3:1HNMR Spectral of compound (3)

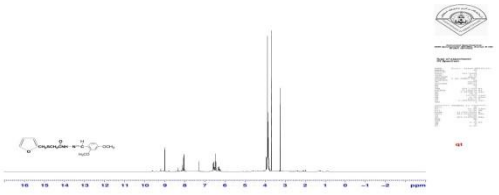


Figure 4:1HNMR Spectral of compound (5)

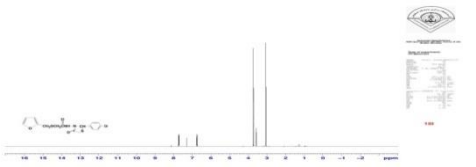


Figure 5:1HNMR Spectral of compound (8)

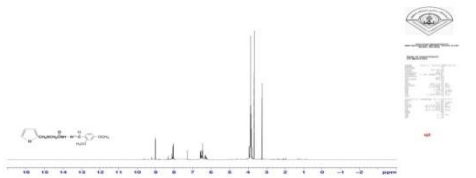


Figure 6: 1HNMR spectral of compound (10)

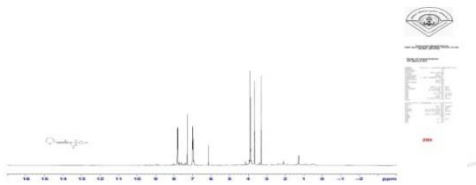


Figure 7:1HNMR Spectral of compound (13)

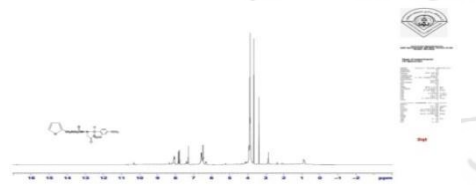


Figure 8:1HNMR Spectral of compound (15)

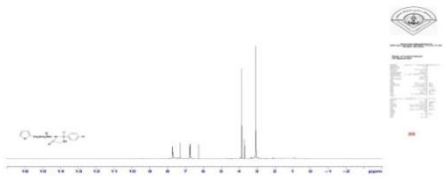


Figure 9:1HNMR Spectral of compound (18)

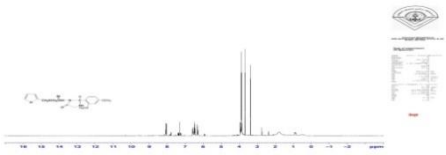


Figure 10:1HNMR Spectral of compound (20)

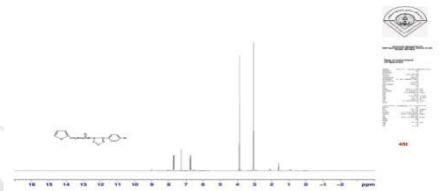


Figure 11:1HNMR Spectral of compound (23)

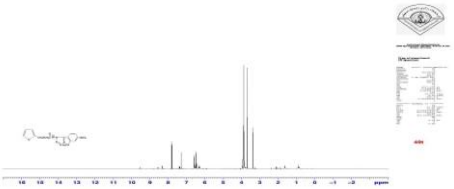
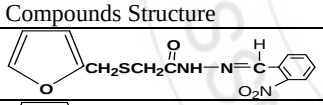
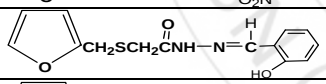
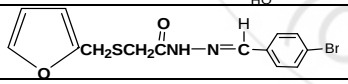
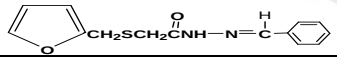
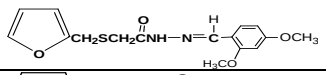
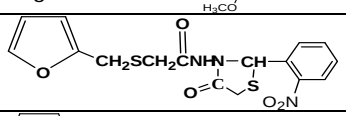
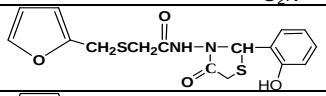
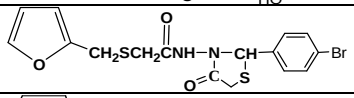
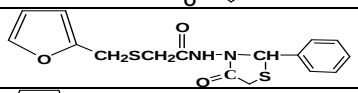
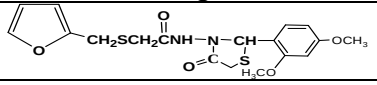


Figure 12:1HNMR Spectral of compound (25)

Table (3-2): FTIR spectral data (cm^{-1}) of compound [1-25]

	Compounds Structure	FTIR spectral data,cm^{-1}
1		ν (N-H)=3080 ,ν (C=O)=1672,ν (C=N)=1627, ν (NO2)= Asym. (1535)and Sym. (1355)
2		ν (N-H)=3180,ν (C=O)=1660 ,ν (C=N)=1602 ν (OH) =3273
3		ν (N-H)=3174,ν (C=O)=1658,ν (C=N)=1604
4		ν (N-H)=3166,ν (C=O)=1664,ν (C=N)=1618
5		ν (N-H)=3174,ν (C=O)=1664,ν (C=N)=1608 ν (CH3) alph. Asym. (2935)and Sym. (2962)
6		ν (N-H)=3396,ν (C=O)ring=1689,ν (C=O)amid=1666, ν (C=C) aromatic=1593, ν (NO2)= Asym. (1521)and Sym. (1346)
7		ν (N-H)=3392,ν (C=O)ring=1683,ν (C=O)amid=1625 , ν (C=C) aromatic=1573 ,ν (OH)=3471
8		ν (N-H)=3423,ν (C=O)ring =1726,ν (C=O)amid=1674, ν (C=C) aromatic=1602
9		ν (N-H)=3182,ν (C=O)ring =1733,ν (C=O)amid=1666, ν (C=C) aromatic=1573
10		ν (N-H)=3178,ν (C=O)=1733ring,ν (C=O)amid=1664, ν (C=C)aromatic =1568,ν (CH_3)= Asym. (2931)and Sym. (2960)

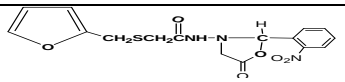
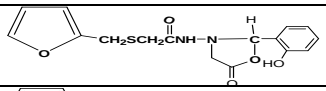
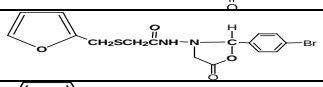
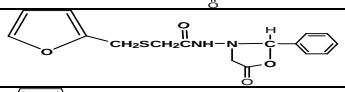
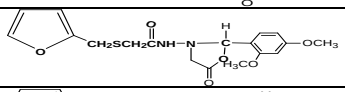
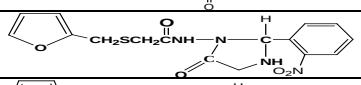
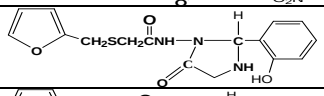
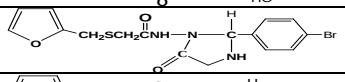
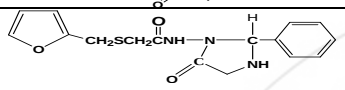
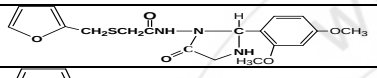
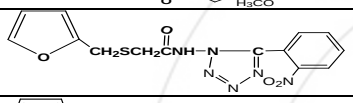
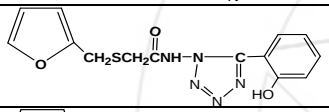
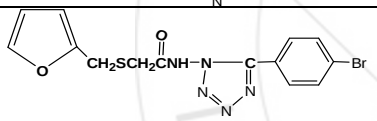
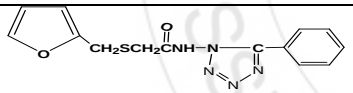
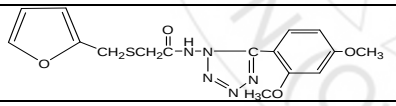
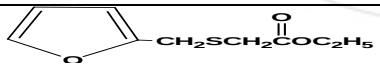
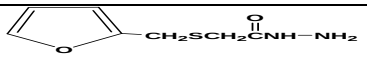
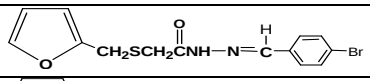
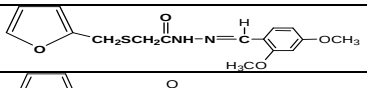
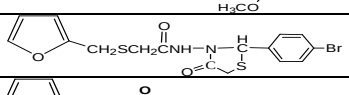
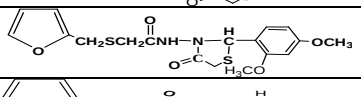
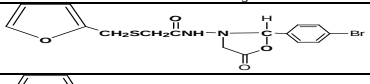
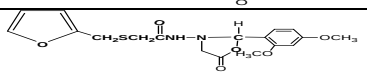
11		ν (N-H)=3088,ν (C=O)ring =1733,ν (C=O)amid=1664 , ν (C=C) aromatic=1569, ν (NO2)= Asym. (1523)and Sym. (1346).
12		ν (N-H)=3215,ν (C=O)ring=1716,ν (C=O)amid=1668 , ν (C=C) aromatic=1576 ,ν (OH)=3398
13		ν (N-H)=3174,ν (C=O)ring=1732,ν (C=O)amid=1683 , ν (C=C) aromatic=1625
14		ν (N-H)=3147,ν (C=O)ring=1768,ν (C=O)amid=1670 , ν (C=C) aromatic=1560
15		ν (NH)=3311,ν (C=O)=1738ring,ν (C=O)amid=1666, ν (C=C)aromatic =1573,ν (CH_3)= Asym. (2921)and Sym. (2954)
16		ν (N-H)=3112,ν (C=O)ring =1689,ν (C=O)amid=1687 , ν (C=C) aromatic=1595, ν (NO2)= Asym. (1519)and Sym. (1344).
17		ν (N-H)=3192,ν (C=O)ring=1719,ν (C=O)amid=1683 , ν (C=C) aromatic=1525 ,ν (OH)=3542
18		ν (N-H)=3170,ν (C=O)ring=1726,ν (C=O)amid=1674 , ν (C=C) aromatic=1562
19		ν (N-H)=3392,ν (C=O)ring=1719,ν (C=O)amid=1683 , ν (C=C) aromatic=1625
20		ν (N-H)=3306,ν (C=O)=1733ring,ν (C=O)amid=1664, ν (C=C)aromatic =1610,ν (CH_3)= Asym. (2931)and Sym. (2960)
21		ν (N-H)=3396,ν (N=N)tetrazol =1490,ν (C=O)amid=1664 , ν (C=N)tetrazol =1608, ν (NO2)= Asym. (1523)and Sym. (1352).
22		ν (N-H)=3396,ν (N=N)tetrazol=1487,ν (C=O)amid=1676 ,ν (C=N)tetrazol =1623
23		ν (N-H)=3392,ν (N=N)=1433,ν (C=O)amid=1662 , ν (C=N)tetrazol =1600
24		ν (N-H)=3392,ν (N=N)tetrazol =1404,ν (C=O)amid=1670 ,ν (C=N)tetrazol =1600
25		ν (N-H)=3306,ν (N=N)tetrazol =1417 , ν (C=O)amid=1666, ν (C=N)tetrazol =1623,ν (CH_3)= Asym. (2921)and Sym. (2975)

Table (3.3): 1H-NMR spectral data (δ ppm) for some compounds

Comp. No.	Structure	^{1}HNMR Spectral data ($^\delta$ppm)
a		1.3 (t,3H,C<u>H</u>$_3$) ; 3.2 (s,2H,S-<u>CH2</u>-C=O); 3.9 (s,2H,C<u>H2</u>-S); 4.2 (q,2H,-C<u>H2</u>-CH_3); (6.1- 7.4) (m,3H,Ar-H)
b		3.25 (s,2H,-S-CH2-C=O) ; 3.7 (d,2H,NH2) ; 3.9 (s,2H,CH2-S); (6.1-7.3) (m,3H,Ar-H); 7,9 (s,1H,N-H)
3		3.1 (s,2H,S-<u>CH2</u>-C=O); 3.9 (s,2H,C<u>H2</u>-S); (6.7- 7.7) (m,7H,Ar-<u>H</u>);8,6 (s,1H,N=C-<u>H</u>); 7.3 (s,1H,N-H)
5		3.2 (s,2H,-S-CH2-C=O);3.7 (s,3H,OCH3) ; 3.9 (s,2H,CH2-S); (6.4-7.3) (m,6H,Ar-H); 8,1 (s,1H,N=C-<u>H</u>); 9 (s,1H,N-H)
8		3.1 (s,2H,S-<u>CH2</u>-C=O); 3.5,3.75 (s,2H,C<u>H2</u>-S); (6.75- 7.3) (m,7H,Ar-<u>H</u>);6,7 (s,1H,N-C-<u>H</u>); 7.3 (s,1H,N-H
9		3.37 (s,2H,-S-CH2-C=O);3.8 (s,3H,OCH3) ; 4 (s,2H,CH2-S); (6.2-7.8) (m,6H,Ar-H); 6,2 (s,1H,N-C-<u>H</u>);7.3 (s,1H,N-H)
13		3.3 (s,2H,-<u>CH2</u>-C=O); 3.7 (s,2H,C<u>H2</u>-N); 3.9 (s,2H,C<u>H2</u>-S); (6.2- 7.8) (m,7H,Ar-<u>H</u>);6,2 (s,1H,N-C-<u>H</u>);7.3 (s,1H,N-H)
15		3.4 (s,2H,-CH2-C=O);3.7 (s,3H,OCH3) ; 3.9 (s,2H,CH2-S); (6.5-7.8) (m,6H,Ar-H); 6,5 (s,1H,N-C-<u>H</u>); 7.3 (s,1H,N-H

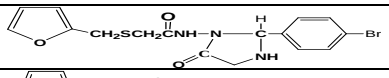
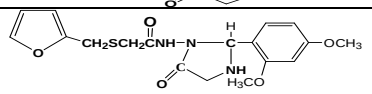
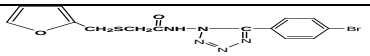
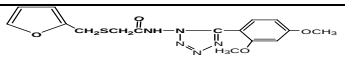
18		3.1 (s,2H,-CH2-C=O); 3.85 (s,2H,CH2-S); (6.25- 7.78) (m,7H,Ar-H);6,25 (s,1H,N-C-H);7.32 (s,1H,N-H)
20		3.4 (s,2H,-CH2-C=O);3.7 (s,3H,OCH3) ; 3.9 (s,2H,CH2-S); (6.5-7.8) (m,6H,Ar-H); 6,5 (s,1H,N-C-H); 7.3 (s,1H,N-H)
23		3.1 (s,2H,-CH2-C=O); 3.9 (s,2H,CH2-S); (6.7-7.8) (m,7H,Ar-H); 7.3 (s,1H,N-H)
25		3.4 (s,2H,-CH2-C=O);3.7 (s,3H,OCH3) ; 3.9 (s,2H,CH2-S); (6.5-7.8) (m,6H,Ar-H); 7.3 (s,1H,N-H)

Table (3-4) : The C.H.N.S analysis ofsome compounds

Comp. NO.	Moleculare Formula	Calculate, (%)				Found, (%)			
		C	H	N	S	C	H	N	S
a	$C_9H_{12}O_3S$	54	6	-	16	53.6	5.4	-	16
b	$C_7H_{10}O_2N_2S$	45	5.37	15.05	17.2	44.9	5.2	14.9	17.1
1	$C_{14}H_{13}O_4N_3S$	52.66	4.07	13.16	10.03	52.5	3.9	13	10
2	$C_{14}H_{14}O_3N_2S$	57.93	4.82	9.65	11.03	58.01	4.7	9.55	11
5	$C_{16}H_{18}O_4N_2S$	57.48	5.38	8.38	9.58	57.46	5.4	8.4	9.56
7	$C_{16}H_{16}O_4N_2S_2$	52.74	4.39	7.69	17.58	52.71	5.4	7.69	17.59
11	$C_{16}H_{15}O_6N_3S$	50.92	3.97	11.14	8.48	50.9	3.94	11.14	8.46
16	$C_{16}H_{16}O_5N_4S$	51.06	4.25	14.89	8.51	51.22	4.1	14.89	8.52
17	$C_{16}H_{17}O_4N_3S$	55.33	4.89	12.1	9.2	55.5	4.51	12.12	9.26
21	$C_{14}H_{12}O_4N_6S$	46.6	3.33	23.33	8.88	46.35	3.91	23.1	9.69

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