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Design and characterization of oxazepine new drivaives

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***Abstract*---**In the presence of ethanol and glacial acetic acids, aniline reacted with aromatic heterocyclic aldehydes such as pyridine-3-carbaldehyde, 1H-pyrrole-2-carbaldehyde, and furan-2-carbaldehyde to generate the imine group known as Schiff bases. Schiff bases IIIA, IIIB, and IIIC are 1-(furan-2-yl)-N-phenylmethanimine, N-phenyl-1-(pyridin-3-yl) methanimine, and N-phenyl-1-(1H-pyrrol-2-yl) methanimine. 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA, 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB ,4-phenyl-3-(1H-pyrrol-2-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVC . These structures of synthetic oxazepine have been characterized by using FTIR, mass spectral, and elemental analyses. The purity quality of the compounds was done using TLC.

***Keywords*---**oxazepine, characterization, design, Schiff bases**.**

Introduction

In the realm of coordination chemistry, Schiff bases are among the most common and important mixed donor systems. Schiff (1884) reported the first preparation of imines, which were made by condensing primary amines with an aldehyde or ketone under specific conditions [1]. Due to the relative ease of preparation, synthetic versatility, and particularly unique property of the C=N group, Schiff bases are considered excellent chelating agents, and their metal complexes have found to exhibt metal complexes.

In addition to the five carbon atoms, 1,3-oxazepine is an unsaturated seven-member heterocyclic ring with an oxygen atom in position 1 and a nitrogen atom in position 3. (Zeid, 2013). Because of their wide range of applications, oxyazepines are essential unsaturated seven-membered heterocyclic rings. The biological activities of 1,3-Oxazepine compounds have been discovered in the research domains as antihistaminic and antiallergic agents (Kubota 2011), hypnotic muscle relaxation (Abdel-Hafez 2008), and anti-inflammatory actions (Abdel-Hafez 2008). (Adnan 2014).

Furthermore, these metal-containing heterocycles have antibacterial and antifungal properties (Serrano-Wu 2002), as well as central depressive (Maysaloon 2014), analgesic (Hallinan 1993), and local anesthetic effects (Hallinan 1993). (Vardanyan 2006) [3] In present work I synthesized new derivatives oxazepine such as 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA, 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB ,4-phenyl-3-(1H-pyrrol-2-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVC and identified by diffrent spectral instrument which is expected to have good biological activity .

Experimental Section

The melting points equipment U.K. and the MS Model: 5973 Agilent Technology (HP) of Mass spectra were used to investigate oxazepine and its novel derivatives. On an infrared Shimandzu spectrophotometer, FT-IR spectra were investigated in the KBr pallet in the 200-4000 cm-1 range, C, H, and N. On a flashing thermo analyzer, elemental equipment analysis was performed.

Synthesis of 1-(furan-2-yl)-N-phenylmethanimine Schiff base IIIA

Preparation of derivatives of 1-(furan-2-yl)-N-phenylmethanimine (Schiff bases) A mixture of aromatic hetero aldehyde furan-2-carbaldehyde (0.01mol) and the compound aniline (0.01mol). dissolved in (30 mL) of absolute ethanol ,were refluxed (75c^{o}) with continuous stirring ,after cooling to room temperature, the precipitate filtered and recrystallized from ethanol, the end of the reaction checked by TLC [4].

Synthesis of N-phenyl-1-(pyridin-3-yl)methanimine Schiff base IIIB

Preparation of derivatives of N-phenyl-1-(pyridin-3-yl)methanimine (Schiff bases) A mixture of aromatic hetero aldehyde pyridine-3-carbaldehyde (0.01mol) and the compound aniline (0.01mol). dissolved in (30 mL) of absolute ethanol ,were refluxed (75 c^{o}) with continuous stirring ,after cooling to room temperature, the precipitate filtered and recrystallized from ethanol, the end of the reaction checked by TLC.

Synthesis of N-phenyl-1-(1H-pyrrol-2-yl)methanimine Schiff base IIIC

Preparation of derivatives of N-phenyl-1-(1H-pyrrol-2-yl)methanimine (Schiff bases) A mixture of aromatic hetero aldehyde 1H-pyrrole-2-carbaldehyde (0.01mol) and the compound aniline (0.01mol). dissolved in (30 mL) of absolute ethanol ,were refluxed (75 c^{o}) with continuous stirring ,after cooling to room temperature, the precipitate filtered and recrystallized from ethanol, the end of the reaction checked by TLC .

Synthesis of 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA

Preparation of 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione by a mixture of (0.01mol) 1-(furan-2-yl)-N-phenylmethanimine Schiff base IIIA which was synthesized before and (0.01mol) of phathalic anhydride for the

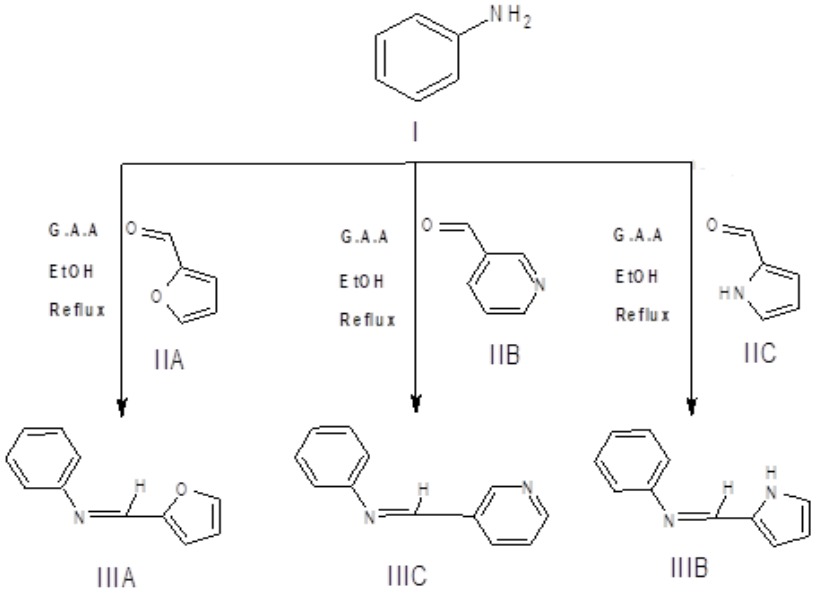
compounds in (50mL) of absolute ethanol was refluxed (75c^{o}) with stirring for 5 hr .Cooling at room temperature, then the precipitate,formed is filtered off and recrystallized from absolute ethanol. The physical properties are listed in table (1)[5,6].

Synthesis of 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB

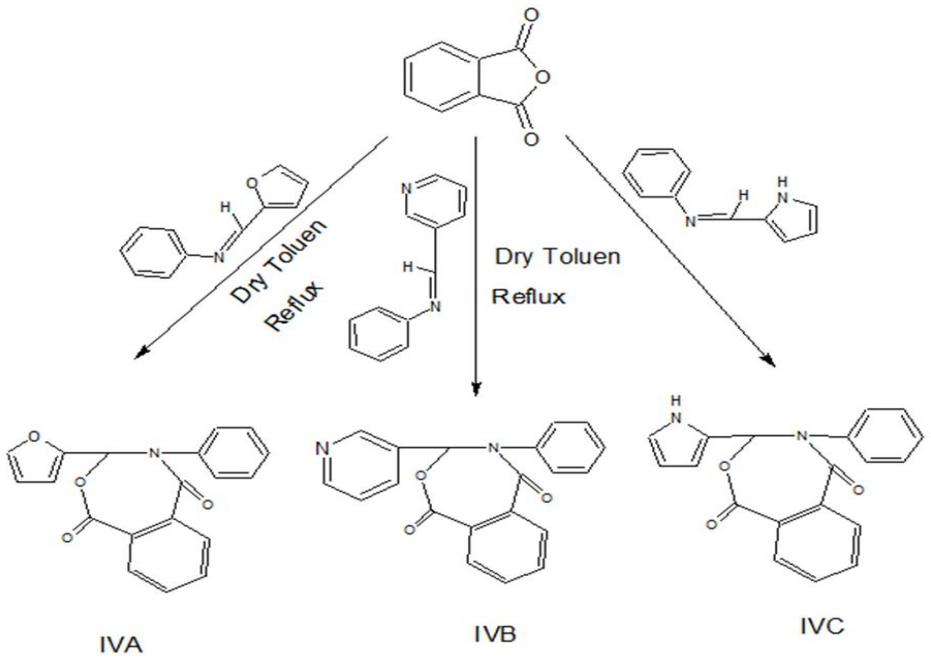
Preparation of IVB by a mixture of (0.01mol) N-phenyl-1-(pyridin-3-yl) methanimine Schiff base IIIB which was synthesized before and (0.01mol) of phathalic anhydride for the compounds in (50mL) of absolute ethanol was refluxed (75c^{o}) with stirring for 5 hr .Cooling at room temperature, then the precipitate,formed is filtered off and recrystallized from absolute ethanol. The physical properties are listed in table (1).

Synthesis of 4-phenyl-3-(1H-pyrrol-2-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVC

Preparation of 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione by a mixture of (0.01mol) 1-(furan-2-yl)-N-phenylmethanimine Schiff bas IVBe IIIA which was synthesized before and (0.01mol) of phathalic anhydride for the compounds in (50mL) of absolute ethanol was refluxed (75c^{o}) with stirring for 5 hr .Cooling at room temperature, then the precipitate,formed is filtered off and recrystallized from absolute ethanol. The physical properties are listed in table (1).



Scheme 1: Synthesis of Schiff base dervatives IIIA , IIIB, IIIC



Scheme 2 : Scheme 1: Synthesis of Oazepine dervatives IVA , IVB, IVC

Table No 1:physiochemical date of synthesized Oazepine dervatives IVA ,IVB, IVC					
Symbol	Molecular formula	M.W(gm/mole)	Color	Melting points /°C	Yield (%)
IVA	$C_{19}H_{13}NO_4$	319	Deep yellow	140-142	72%
IVB	$C_{20}H_{14}N_2O_3$	330	Deep yellow	144-146	75%
IVC	$C_{19}H_{14}N_2O_3$	318	Brown	142-144	71%

Table No 2 :elemental analysis of synthesized Oazepine dervatives IVA , IVB, IVC				
		C	H	N
IVA	Theoretical Data	52.99%	3.49%	20.17%
	practical Data	52.83%	3.36%	20.03%
IVB	Theoretical Data	53.16%	3.82%	17.71%
	practical Data	53.04%	3.77%	17.59%
IVC	Theoretical Data	56.13%	4.12%	16.36%
	practical Data	56.03%	4.01%	16.27%

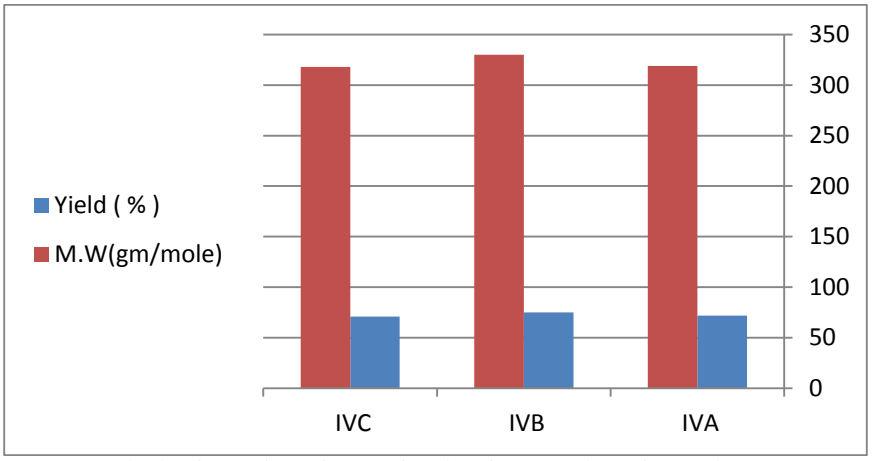


Figure No 1 :statistical study of synthesized Oazepine dervatives IVA , IVB, IVC

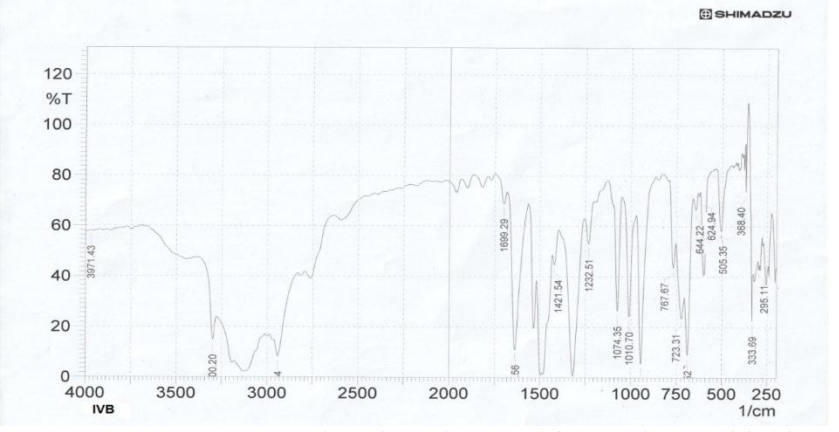


Figure No 2 : Ft-IR spectra of 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB

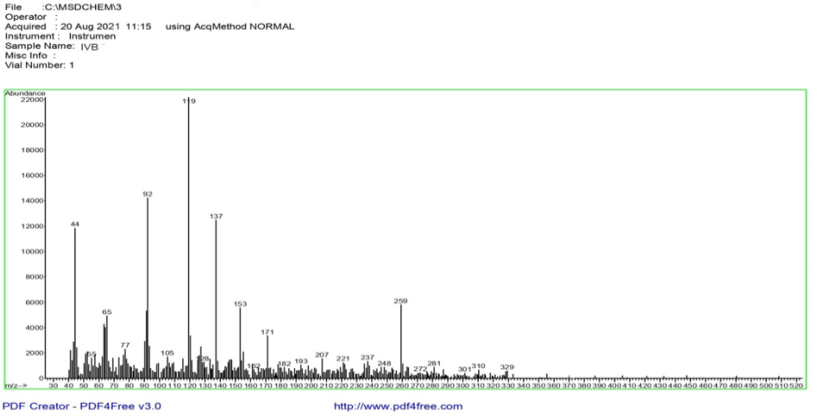


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Figure No 3 : Mass spectra of 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB.

Results and Discussion

IR and mass spectra of an oxazepine derivative synthesized 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVC, 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA, 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4 Table 1 shows the molecular formula and melting temperatures of synthesized compounds, as well as yield %, color, and molecular weight. Table 2 shows the elemental analysis of the synthesized compounds IVA, IVB, and IVC, which were found to be in good agreement with the recommended design structural formula. as seen in Figure 1 Tables 1 and 2 [7,8] provide all of the data. [7,8].

FTIR (KBr, cm-1) of 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA showed 3115 (C-H) Aromatic 2910 (C-H)Ali, 1738 (C=O) ester and 1695 (C=O) amide respectively . While FTIR (KBr, cm-1) of 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB showed 3105 (C-H) Aromatic 2905 (C-H)Ali, 1725 (C=O) ester, 1699 (C=O) amide , and 1605 (C=N) respectively as show in (Fig 2). While FTIR (KBr, cm-1) of 4-phenyl-3-(1H-pyrrol-2-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVC showed 3015 (C-H) Aromatic 2925 (C-H)Ali, 1718 (C=O) ester, 1685 (C=O) amide and 3420 (N-H) respectively[9,10] .

The mass spectra of synthesized target compounds of 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA showd molecular ion peaks at 319,241,175,130,105,92,77,67,64 in mass spectral which are blelong to the following molecular ion fragment $C_{19}H_{13}NO_4$, $C_{13}H_7NO_4$, $C_{14}H_7NO_3$, $C_{14}H_9NO_2$, C_9H_6O, $C_{14}H_9NO$ C_8H_8, C_7H_7, C_6H_5, $C_9H_5NO_3$, C_4H_3O, C_5H_5 as show in (Fig 3).the ion fragment mass data confirmed the composition of synthesized oxazepine IVA [11.12] .

The mass spectra of synthesized target compounds 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB showd molecular ion peaks at 329, 250 ,237,223,208,130,105,92,77,64 in mass spectral which are blelong to the following molecular ion fragment $C_{20}H_{14}N_2O_3$, $C_9H_5NO_3$, $C_{14}H_9N_2O_3$ M+2, $C_{14}H_7NO_3$, $C_{14}H_9NO_2$, C_9H_6O , $C_{14}H_9NO$ C_8H_8, C_7H_7, C_6H_5, C_5H_5 as show in (Fig 3).the ion fragment mass data confirmed the composition of synthesized oxazepine IVB .[13]

The mass spectra of synthesized target compounds 4-phenyl-3-(1H-pyrrol-2-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione showd molecular ion peaks at 318,240,175,130,105,92,77,66,64 in mass spectral which are blelong to the following molecular ion fragment $C_{19}H_{14}N_2O_3$, $C_{13}H_8N_2O_3$, $C_{14}H_7NO_3$, $C_{14}H_9NO_2$, C_9H_6O, $C_{14}H_9NO$ C_8H_8, C_7H_7, C_6H_5, $C_9H_5NO_3$, C_4H_4N, C_5H_5 as show in (Fig 3).the ion fragment mass data confirmed the composition of synthesized oxazepine IVC [14].

Conclusion

In the present study, Synthesis of 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA , Synthesis of 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB and Synthesis of 4-phenyl-3-(1H-pyrrol-2-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVC synthesized and Characterized by

different physical feature like melting point and colour also by different spectral technique like IR, Mass spectra ,also instrumentally by elemental analyses C, H, N.

IR spectra showed five important band on 3105, 2905, 1725, 1699 and 1605 respectively as show in (Fig 2) which were corresponding to (C-H) aromatic and (C-H) aliphatic and also C=O of ester, C=O of amide and C=N of pyridine ring of IVB .that is good support to formation of oxazepine derivatives. The mass fragment ion showed ion peak at. The mass spectra of synthesized target compounds showd molecular ion peaks at 319,329 and 318 in mass spectral which are blelong to the following molecular ion of the synthesized strucutre of 3-(furan-2-yl)-4-phenyl-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVA , Synthesis of 4-phenyl-3-(pyridin-3-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVB and Synthesis of 4-phenyl-3-(1H-pyrrol-2-yl)-3,4-dihydro-2,4-benzoxazepine-1,5-dione IVC , as show in (Fig 3).the ion fragment mass data confirmed the composition of synthesized oxazepine IVB .

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