Synthesis and Identification some of heterocyclic compounds from 2-Aminobenzimidazole

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Abstract

This reserch involved hetrocyclic compounds such as (Thiazolidine derivatives , imidazolidin derivatives,oxazole derivatives, imidazole derivatives and pyridine derivatives) were prepared by reaction 2-aminobenzaldehyde with benzaldehyde derivatives (4-dimethylaminobenzaldehyde, furfural,vanillin) to get shiff base (1-3) , N-(4-(dimethylamino) benzylidene)-1H-benzo[d]imidazol-2-amine(1), N-(furan-2-ylmethylene)-1H-benzo[d]imidazol-2-amine(2), 4-(((1H-benzo[d]imidazol-2-yl) imino) methyl)-2-methoxyphenol (3) .

The cyclization of (1-3) with α-aminoacid (glycine) give the corresponding 3-(1H-benzo[d] imidazol-2-yl)-2-(4-(dimethylamino) phenyl) imidazolidin-4-one (4), 3-(1H-benzo[d] imidazol-2-yl)-2-(furan-2-yl) imidazolidin-4-one (5) , 3-(1H-benzo[d] imidazol-2-yl)-2-(4-hydroxy-3-methoxyphenyl) imidazolidin-4-one (6) , and when cyclization of (1-3) with thioglycollicacid give the corresponding 3-(1H-benzo[d] imidazol-2-yl)-2-(4-(dimethylamino) phenyl) thiazolidin-4-one (7), 3-(1H-benzo[d]imidazol-2-yl)-2-(furan-2-yl) thiazolidin-4-one(8), 3-(1H-benzo[d] imidazol-2-yl) -2-(4-hydroxy-3-methoxyphenyl) thiazolidin-4-one (9) .

As well as the reaction of 2 - Amino benzoimidazole with chloro acetyl chloride to get N-(1H-benzo[d] imidazol-2-yl)-2-chloroacetamide which reacts with urea , thiourea , thiosemicarbazide, 2-aminobenzimidazole, 2-aminopyridine give the corresponding N5-(1H-benzo[d] imidazol-2-yl) oxazole-2,5-diamine (11),N5-(1H-benzo[d] imidazol-2-yl) thiazole-2,5-diamine(12),N-(1H-benzo[d] imidazol-2-yl)-2-(2-carbamothioylhydrazinyl) acetamide(13),2-((1H-benzo[d] imidazol-2-yl) amino)-N-(1H-benzo[d] imidazol-2-yl) acetamide (14) , N-(1H-benzo[d] imidazol-2-yl)-2-(pyridin-2-ylamino) acetamide (15) .
.All this compounds characterized by means of FT- IR ,and some of the compoundesby means ^{1}H-NMR,and 13C-NMR and follow reaction by R_f - TLC and Measure ment melting point .

Key words:- 2-aminobenzoimidazole ,Thiazolidin , Imidazolidin, oxazole.

الخلاصة

تضمن البحث تحضير مركبات حلقيه غير متجانسة مثل (مشتقات اميدازولدين, مشتقات ثازولدين ,مشتقات اوكسازول ,مشتقات اميدازول ,مشتقات بريدين) وذلك من تفاعل 2- امينوبنزواميدازول مع مشتقات البنزلديهايد (4-ثنائي مثيل امينو بنزلديهايد ,فورفورال ,فانلين) لتحضيرقواعد شف (1-3) وهي نتروجين- (4-(ثنائي مثل امينو) بنزلدين) -1هيدروجين -بنزواميدازول -2-امين (1) , نتروجين -(فيوران-2ايل مثلين)-اهيدروجين-بنزواميدازول-2-امين)(2) و4-((((1هيدروجين-بنزواميدازل-2-ايل) امينو)مثيل)-2-ميتوكسي فينول (3). تم تفاعل هذه المركبات مع الكلايسين مره لنحصل على مشتقات الاميدازولدين (4-6) وهي 3-(1 هيدروجين-بنزواميدازول 2-ايل) -2- (4-(ثنائي مثيل امينو)فنيل)اميدازولدين -4-اون(4) , 3-(1هيدروجين-اميدازول -2-ايل) -2-(فيوران-2-ايل)اميدازولدين -4- اون (5) و3-(1 هيدروجين-بنزواميدازول 2-ايل) -2- (4-هيدروكسي -3- ميثوكسي فنيل)اميدازولدين -4-اون (6) . كذلك تفاعل (1-3) مع حامض الثايوكلايكول لنحصل على مشتقات الثايزولدين(7-9) وهي 3-(1 هيدروجين-بنزواميدازول 2-ايل) -2- (4-(ثنائي مثيل امينو)فنيل)ثايازولدين -4-اون(7) , 3-(1هيدروجين-اميدازول -2-ايل) -2-(فيوران-2-ايل)ثايازولدين -4- اون (8) و3-(1 هيدروجين-بنزواميدازول 2-ايل) -2- (4-هيدروكسي -3- ميثوكسي فنيل)ثايازولدين -4-اون(9) . كذلك تفاعل 2- امينو بنزواميدازول مع كلورواسيتايل كلورايد لنحصل على نتروجين-_اهيدروجين-بنزواميدازول-2-ايل)-2-كلورواستمايد(10) ,الذي يتفاعل مع كل من اليوريا والثايويوريا وثايوسيماكاربازايد و2-امينوبنزو اميدازول و2-امينو بريدين لنحصل بالمقابل على نتروجين(1هيدروجين-بنزواميداول-2-ايل)اوكسازول-2و5-ثنائي امين(11) , نتروجين-(ا-هيدروجين-بنزواميدازول-2-ايل)ثايازول-2و5-ثنائي-5,2-ثنائي امين (12) و نتروجين-(1هيدروجين-بنزواميدازول-2-ايل)-2-(2-كاربراميثويل هيدرازيل) استمايد(13) , 2-((1هيدروجين-بنزو اميدازول-2-ايل)امينو)-نتروجين-(1هيدروجين-بنزواميدازول-2-ايل)استمايد (14) , نتروجين-(1هيدروجين-بنزواميدازول-2-ايل)-2-(بريدين-2ايل-امينو)استمايد (15).

كل هذه المركبات تم تشخيصها بوساطة مطيافيه الاشعه تحت الحمراء وبعضها بوساطة مطيافية الرنين النووي المغناطيسي و متابعة التفاعل بكروموتوغرافيا الطبقة الرقيقه وقياس درجة الانصهار C-13

الكلمات المفتاحية :- المركبات الحلقيه غير المتجانسة ,2-امينوبنزواميدازول,ثايوزولدين , اميدازولدين واوكسازول.

Introduction

Benzimidazole derivatives play important role in medical field with many pharmacological activities such as antimicrobial, antiviral, antidiabetic and anticancer activity[1-3]. Therefore substituted benzimidazoles have attracted the interest of various research group, especially since it has been reported that the influence of the substitution at 1,2 and 5-positions is very important for their pharmacological effect[4,5]. the benzimidazole moiety express significant activity against several viruses such as HIV4, Herpes(HSV-1) 5 and influenza6. Bisbenzimidazoleis DNA-

minor grove binding agents possessing anti-tumour activity[6,7].
imidazolidin-dione are belongs to heterocyclic compound, which has a wide range of biological and pharmacological properties such as antimicrobial activity (antifungal, antibacterial), antitumor, antiinflammatry , anti HIV, anti-hypertensive, hydantoin exhibits diverse biological activities, such as anticonvulsant, antifungal activities, antithyroidal, antiviral, , tuber culosis, anti arrhythmic and anti convulsant [8-10].

The versatile uses of thiazolidinones as anaesthetics, anti-convulsants, amoebicides, hypotensive and tuberculostatic agents have stimulated a considerable interest to explore the possible synthesis of new potential compounds in which the thiazolidinone ring is fused with another biologically active nucleus. With a view in achieving such a system, the thiazolidine was fused with benzimidazole. Benzimidazole nucleus was chosen because certain 2-amino benzimidazole were found to possess some anti-viral activity[11-15].

The oxazole moiety was chosen for conducting property studies due to the significant applications like versatile biological activities , application as important precursors in organic transformations , fluorescent whitening agents , and scintillating compounds[16].
A large number of natural products, in particular from the marine environment, contain thiazole, oxazole, heterocycles. In many cases, promising anti-tumor,antibacterial, anti-viral,anti-malaria and anthelmintic activities have been identified forthese compounds[17-19].

Experimental Apparatus

(FTIR)Spectra(4000-400cm-1)in KBr disk were recorded on aSHIMADZU FTIR-8400S fourier.transform. melting point were measured using Stuart, UK.
^{1}HNMR and ^{13}C-NMR were recorded on fourier transformation bruker spectrometer ,operating at (400MHz) with (DMSO-ds) measurments were made at Department of chemistry ,kashan university .Iran.

General method of synthesis of schiff bases compounds (1-3)[20]

A mixture of equimolar quantities (0.01mol) of aromatic benzaldehyde and 2-aminobenzoimidazol was refluxed for 20 min in 30 ml of ethanol. The reaction mixture was cooled and kept for (24 hs) . The crystals found was filtered , dried and recrystallized from ethanol to give compounds (1-3) .

General method of synthesis of imidazolidin-4-one derivative (4-6)

A mixture of schiff bases(1-3) (0.001mol) dissolved in THF (15mL) and glycine (0.001mol)was dissolved in THF (15mL)and refluxed for 24 hs.The reaction was then cooled and the resulting final (4-6) ,recrystallized from ethanol.

General method of synthesis of thiazolidinones (7-9)

A mixture of schiff bases (1-3) (0.001mol)and thioglycollic acid (0.001mol) dissolved in 1,4 dioxane (20mL), anhydrous zinc chloride(0.7gm)was added and refluxed for 8 h. The reaction was then cooled and the resulting solid was washed with sodium bicarbonate solution and final (7-9) recrystallized from absolute ethanol.

method of synthesis of (10)[21]

Chloroacetyl chloride (0.01 mol) was added to a solution of (0.01mol) 2-amino benzo imidazol in benzene (20 ml). The

mixture was stirred at room temperature for 2-3 hours and poured onto ice. The separated solid was filtered, washed with water, dried and recrystallized from aqueous ethanol

method of synthesis of (11)[22]

To a solution of (10) (3.5 mmol) in absolute ethanol (60 mL), urea (3.5 mmol) was added. The mixture was heated at reflux for 30 min. cooling after netruleis by 10% NaOH, precipitate was collected and recrystallized from ethanol, to give (11) .

method of synthesis of (12)[22]

To a solution of (10) (3.5 mmol) in absolute ethanol (60 mL), thiourea (3.5 mmol) was added. The mixture was heated at reflux for 30 min. After cooling, the precipitate was collected and recrystallized from ethanol–10 % sodium hydroxide, to give(12)

method of synthesis of (13)

(0.01 mole) of (10) in 30 ml ethanol was added to (0.01 mole) thiosemicarbazide
and Drops of pyridine , The mixture was stirred at room temperature for 24 hours ,left it at room temperature for 24 hs. The precipitate was filtered off and then recrystallized from ethanol.

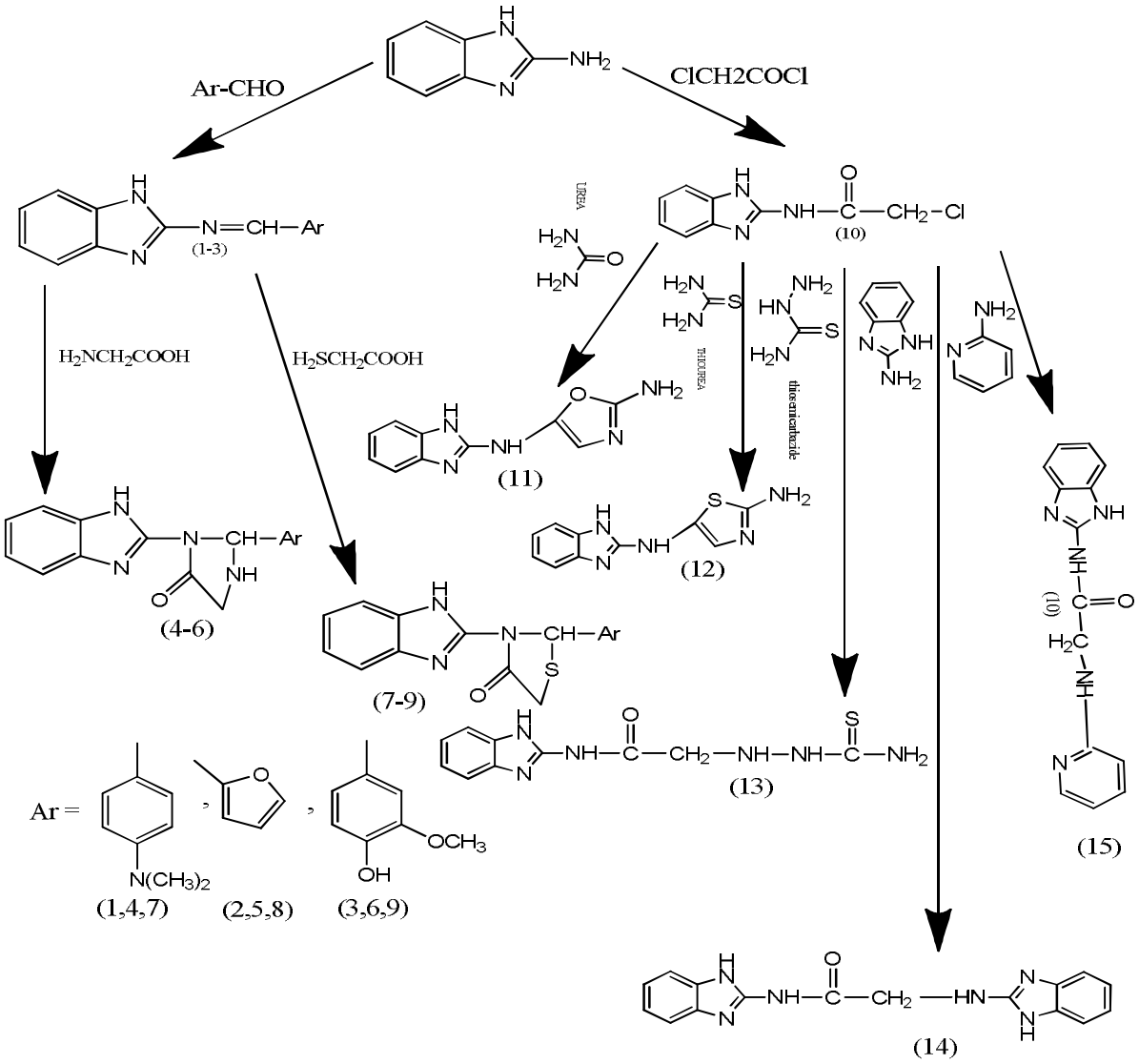
method of synthesis of (14)[23]

To compound (10)(0.001 mole) dissolved in 20m1, ethanol. 2-aminobenzoimidazole (0.00lmole) was added gradually. When addition was complete reaction mixture was reflex for 6 hr**.** After the reaction excesses of ethanol and aryl amine were recovered distillation. The residue was washed with sodium bicarbonate to remove the acid impurities and finally with water. The product was crystallized from a ethanol .

method of synthesis of (15)[23]

To compound (10)(0.001 mole) dissolved in 20m1, ethanol. 2-aminopyridine (0.00lmole) was added gradually. When addition was complete reaction mixture was reflex for 6 hr**.** After the reaction excesses of ethanol and aryl amine were recovered distillation. The residue was washed with sodium bicarbonate to remove the acid impurities and finally with water. The product was crystallized from ethanol .

Schem1



Results and Discussion

compound (1) N-(4-(dimethylamino)benzylidene)-1H-benzo[d]imidazol-2-amine

This compound was obtained as yellow solid yield 90.86%,R_f =0.87, M.P (263)^{O}C.

The infrared spectrum data of compound (1) show absorption at (3055) cm^{-1} for (Ar-H),(3309) cm^{-1} (N-H),(1650) cm^{-1} (C=N),and show new band at (2923) for (C-H)CH_3.

The^{1}H-NMR(DMSO) spectrum data of compound (1) show δ:6.17-7.6(m , 8H , Ar-H) , 9.21 (m , 1H , NH) ,7.8 (m , 1H,CH) , 3.6 (m,6H, CH_3) .

The^{13}C-NMR(DMSO) spectrum data of compound (1) show δ:158.6 (C10) , 156.7 (C2) ,155.8(C14) , 154.8(C8,C9) , 133.1(C12,C16) , 124.07(C9) ,

120.8(C5,C6) , 113.1(C13,C15) , 112.6 (C2,C5) ,22.9 (C17,C18) .

compound (2)

N-(furan-2-ylmethylene)-1H-benzo [d] imidazol-2-amine was obtained as brown solid yield 63% , Rf =0.39 , M.P(174)^{O}C. The infrared spectrum data of compound (2) show absorption at (3055) cm^{-1} for (Ar-H),(3379) cm^{-1} (N-H), (1681) cm^{-1} (C=N),and show band at (1218) for (C-O-C).

compound (3)

4-(((1H-benzo[d]imidazol-2-yl) imino)methyl)-2-methoxyphenol was obtained as orang solid yield 35%,Rf =0.66 ,M.P (81)^{O}C. The infrared spectrum data of compound (3)show absorption at (3062) cm^{-1} for (Ar-H), (3363)cm^{-1} (N-H) ,(1681)cm^{-1} (C=N),and show band at (2877-2931) for (C-H)CH_3,(1234) cm^{-1} for (C-O) C-OH ,(1272) cm^{-1} (C-O) Ph-O-CH_3.

The^{1}H-NMR(DMSO) spectrum data of compound (3) show δ:6.8-8.3(m , 7H , Ar-H) , 9.7 (m , 1H , NH) ,9.3 (m , 1H,CH),3.5(m,6H, CH_3) , 9.2(m,1H,OH).

The^{13}C-NMR(DMSO) spectrum data of compound (3) show δ:158.01 (C10) , 156.5 (C2) ,155.03(C14) , 153.6(C13) , 149.8(C9,C8),139.9(C11), 130.1(C5,C6) , 127.8 (C16),121.2 (C7,C4) , 117 (C15) , 112.1(C12), 66.5(C17) .

Table (1) infrared spectrum data for(1,2,3) compounds

Comp.	υAr-H arom.	υN-H	υC=N	υC-H aleph.	υOH	υArOCH$_3$ CO
1	3055	3309	1650	2923	-	-
2	3055	3379	1681	-		
3	3062	3363	1681	2877-2931	3349	1257

compound (4)

3-(1H-benzo[d]imidazol-2-yl)-2-(4-(dimethylamino)phenyl)imidazolidin-4-one (4) as yellow solid, yield 65.7% ,Rf =0.8 , M.P(186)^{O}C.

The infrared spectrum data of compound (4)show absorption at (3050)cm^{-1} for (Ar-H),(3150) cm^{-1} (N-H),(1681)cm^{-1}(C=N),and show band at(2970)$cm^{-1}$for (C-H)CH_3, and(1690) cm^{-1} for(C=O) .

compound (5) 3-(1H-benzo[d]imidazol-2-yl)-2-(furan-2-yl)imidazolidin-4-one

as Purple solid, yield 65% ,Rf =0.56 , M.P(109)^{O}C.

The infrared spectrum data of compound (5)show absorption at (3070)cm^{-1} for (Ar-H),(3363) cm^{-1} (N-H),(1635)cm^{-1}(C=N),(1712) cm^{-1} for(C=O), and show band at (1218) for (C-O).

compound(6)

3-(1H-benzo[d] imidazol-2-yl)-2-(4-hydroxy-3-methoxyphenyl)imidazolidin-4-oneas Purple solid, yield 66.6% ,Rf =0.82 , M.P(102)^{O}C.

The infrared spectrum data of compound (6) show absorption at (3070) cm^{-1} for (Ar-H),(3163) cm^{-1} (N-H),(1681)cm^{-1}(C=N),and show band at (2970) for (C-H)CH_3,(1226) cm^{-1} for (C-O) C-OH ,(1234) cm^{-1} (C-O) Ph-O-CH_3.),(1702) cm^{-1} for(C=O).

Table (2) infrared spectrum data for imidazolidn-4-one derivatives compounds (4-6) cm^{-1}

Comp.	υAr-H	υN-H	υC=N	υC-H aleph.	υC=O	υOH	υArOCH3 CO
4	3050	3150	1681	2970	1690		
5	3070	3363	1635	-	1712		
6	3070	3163	1681	2970	1690	3346	1234

compound (7)

3-(1H-benzo[d]imidazol-2-yl)-2-(4-(dimethylamino)phenyl)thiazolidin-4-one as yellow solid, yield 76.6% ,Rf =0.65 , M.P(123)^{O}C.

The infrared spectrum data of compound (4)show absorption at (3070)cm^{-1} for (Ar-H),(3332) cm^{-1} (N-H),(1666)cm^{-1}(C=N),and show band at(2916)$cm^{-1}$for (C-H)CH_3, and(1681) cm^{-1} for(C=O) .

ompound (8) 3-(1H-benzo[d]imidazol-2-yl)-2-(furan-2-yl)imidazolidin-4-one

as yellow solid, yield 98% ,Rf =0.64 , M.P(170)^{O}C.

The infrared spectrum data of compound (8)show absorption at (3070)cm^{-1} for (Ar-H),(3332) cm^{-1} (N-H),(1650)cm^{-1}(C=N),(1712) cm^{-1} for(C=O), and show band at (1218) for (C-O).

compound (9)

3-(1H-benzo[d] imidazol-2-yl)-2-(4-hydroxy-3-methoxyphenyl) thiazolidin-4-one as white seram, yield 76.6% ,Rf =0.7 , M.P.

The infrared spectrum data of compound (6) show absorption at (3070) cm^{-1} for (Ar-H), (3379)cm^{-1} (N-H) ,(1681)cm^{-1}(C=N),and show band at (2962) for (C-H)CH_3,(1208) cm^{-1} for (C-O) C-OH ,(1026) cm^{-1} (C-O) Ph-O-CH_3.),(1712) cm^{-1} for (C=O)and (3502)cm^{-1} for(OH) .

The ^{1}H-NMR(DMSO) spectrum data of compound (9) show δ:6.7-7.3(m , 7H , Ar-H) , 9.4 (s , 1H , NH) ,3.7 (m , 1H,CH) , 3.4-3.6(s,2H,CH2),3.1 (m,6H, CH_3) , 5.1(m,1H,OH).

Table(3)infrared spectrum data for imidazolidn-4-one derivatives compounds (7-9) cm^{-1}

Comp.	υAr-H	υN-H	υC=N	υC-H aleph.	υC=O	υOH	υArOCH3 CO	υC-O
7	3070	3332	1666	2916	1681	-	-	-
8	3070	3332	1650	-	1712	-	-	1026
9	3070	3379	1618	2962	1712	3502	1265	1026

compound (10)

N-(1H-benzo[d] imidazol-2-yl)-2-chloroacetamide as Green solid, yield 54.5 ,Rf =0.56 , M.P(198)^{O}C.

The infrared spectrum data of compound (10) show absorption at (3078) cm^{-1} for (Ar-H),(1620) cm^{-1} (C=N),and show new band at (2877-2993) for (C-H)CH_2 , (1689) cm^{-1} for(C=O) and (740) Cm^{-1} for (C-Cl),(3147)Cm^{-1} for (N-H) , (1560) Cm^{-1} for (C=C)

The^{1}H-NMR(DMSO) spectrum data of compound (10) show δ:6.2-7.4(m , 4H , Ar-H) , 11 (s , 1H , NH) , 3.35(m,2H,CH2), 4.3(m,1H,NH).

The ^{13}C-NMR(DMSO) spectrum data of compound (10) show δ:148.5 (C10) , 136.8 (C2) , 123.04 (C9,C8) , 45.07(C11) , 121.9(C5,C6), 113.02(C4,C7) .

compound (11)

N5-(1H-benzo[d] imidazol-2-yl) oxazole-2,5-diamine as orang solid, yield =92% , Rf = 0.5 , M.P(266)^{O}C.

The infrared spectrum data of compound (11) show absorption at (3070) cm^{-1} for (Ar-H),(3379) cm^{-1} (N-H) overlap with absorption of NH_2 and show band at (1272)for C-O , (1650)Cm^{-1} for (C=N) , (1604) Cm^{-1} for (C=C)

The ^{1}H-NMR(DMSO) spectrum data of compound (11) show δ:6.3-7.4(m , 5H , Ar-H) , 11.1 (s , 1H , NH) , 5. 5(m,2H,NH2), 4.1(m,1H,NH).

compound (12)

N5-(1H-benzo[d]imidazol-2-yl) thiazole -2,5-diamine as white solid, yield =72.7% ,Rf =0.57 , M.P(70)^{O}C.

The infrared spectrum data of compound (12) show absorption at (3070) cm^{-1} for (Ar-H),(3147) cm^{-1} (N-H) ,(3350) cm^{-1} for(N-H) for NH_2,(1666) cm^{-1} for (C=C) , (1681) cm^{-1} for (C=N)

compound(13)

N5N-(1H-benzo[d]imidazol-2-yl)-2-(2-carbamothioylhydrazinyl) acetamide as Brown solid, yield =67.79% ,Rf =0.54 , M.P(189)^{O}C.

The infrared spectrum data of compound (13) show absorption at (3070) cm^{-1} for (Ar-H),(3132) cm^{-1} for (N-H) imidazol and show new band at (3360) for NH_2,(1257) for C=S , (2923) for (C-H)CH_2 , (1697)for (C=O) , ,(1620) cm^{-1} for (C=C) , (1681) cm^{-1} for (C=N)

compound(14)

2-((1H-benzo[d]imidazol-2-yl)amino)-N-(1H-benzo[d]imidazol-2-yl) acetamide as Green solid, yield =75.8% ,Rf =0.6 , M.P(162)^{O}C.

The infrared spectrum data of compound (14) show absorption at (3001) cm^{-1} for (Ar-H),(3147) cm^{-1} (N-H),and show new band at (1689) cm^{-1} for C=O ,(1218) cm^{-1} for C-O , (2877-2939) cm^{-1} for (C-H)CH_2,(1620) cm^{-1} for (C=C) , (1635) cm^{-1} for (C=N)

compound(15)

N-(1H-benzo [d]imidazol-2-yl)-2-(pyridin-2-ylamino)acetamide as Brown solid, yield =70% ,Rf =0.34 , M.P(189)^{O}C.

The infrared spectrum data of compound (14) show absorption at (3078) cm^{-1} for (Ar-H),(3178) cm^{-1} (N-H)and show new band at (1689) cm^{-1} for C=O ,(1226) cm^{-1} for C-O , (2931) cm^{-1} for (C-H)CH_2,(1592) cm^{-1} for (C=C) , (1650) cm^{-1} for (C=N)).

Table(4)infrared spectrum data for(10-15) compoundscm^{-1}

Comp.	υAr-H	υN-H Imidazol	υC-H aleph.	υC=O	NH_2	C=S	υC-Cl
10	3078	3147	2939	1689	-	-	740
11	3078		-	-	3379	-	-
12	3070	3147			3350		
13	3070	3132	2923		3360	1257	
14	3001	3147	2939	1689			
15	3078	3178	2931	1689			

Table(5):- Analytical and physical data of compounds .

No.	Molecular formula	Color	M.P°C	Yield%	R_f
1	$C_{16}H_{16}N_4$ (264.325)	yellow	263	90.86	0.87
2	$C_{12}H_9N_3O$ (211.219)	Brown	174	63	0.39
3	$C_{15}H_{13}N_3O_2$ (267.283)	orang	81	35%	0.66
4	$C_{18}H_{19}N_5O$ (321.37)	yellow	186	65.7	0.8
5	$C_{14}H_{12}N_4O_2$ (268.807)	purple	109	65	0.56
6	$C_{17}H_{16}N_4O_3$ (324.334)	purple	102	66.6	0.82
7	$C_{18}H_{18}N_4OS$ (338.42)	yellow	123	76.6	0.65
8	$C_{14}H_{11}N_3O_2S$ (285.32)	yellow	170	98	0.64
9	$C_{17}H_{15}N_3O_3S$ (341.38)	white	seram	76.6	0.7
10	$C_9H_8N_3OCl$ (209.632)	Green	198	54.5	0.56
11	$C_{10}H_9N_5O$ (215.211)	orang	266	92	0.5
12	$C_{10}H_9N_5S$ (231.277)	white	70	72.7	0.57
13	$C_{10}H_{12}N_6OS$ (264.079)	Brown	seram	67.79	0.54
14	$C_{16}H_{14}N_6O$ (306.322)	Green	162	75.8	0.6
15	$C_{14}H_{13}N_5O$ (267.286)	Brown	189	70	0.34

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