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Synthesis, Identification of Some New 1, 2, 4-triazole Derivatives from 2-(4-methoxyphenyl)-3-ethyl acetate -4(3H) - quinazolinone and Evaluation Anti-Oxidant Activity.

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Abstract

In this study, novel derivatives have been synthesized for 1,2,4-triazole-quinazolinone compounds. The intermediate compound, amic acid **1**, was prepared through the reaction of anthranilic acid with para-methoxybenzoyl chloride. The compound benzoxazinone **2** is prepared by reacting amic acid with acetic anhydride, which upon esterification is carried out using ethylglycinate hydrochloride. Ester derivative **3** was obtained. The first line of research involved reacting the ester derivative 3 with (semicarbazide, thiosemicarbazide, and phenylthiosemicarbazide, phenylthiosemicarbazide) respectively to give derivatives **5-8**. Compounds **5-8** were cyclized in alkaline medium (2N-NaOH) gave 1, 2, 4-triazole derivatives **9-12**, respectively. Alternatively, compound **4** was reacted with CS_2 in an alkaline medium (20% KOH) to produce the potassium salt **13**. This compound then directly reacted with aqueous hydrazine to yield compound **14**. The new compositions prepared were proven using spectroscopic techniques [FT-IR, 1H-NMR, 13C-NMR,]. The last part of this research in which, these materials were tested **5, 9, 11, 12, 13, 14** for antioxidant activity using DPPH radical scavenging activity technology.

Keywords: anthranilic, Semicarbazid, Thiosemicarbazide, 1, 2, 4-triazole, Anti-oxidant

تحضير وتشخيص بعض مشتقات 1، 2، 4 ترايازول الجديدة من 2-(4-ميثوكسي فينيل) -3-ايثيل أسيتات -4(3H) كينازولينون وتقييم الفعالية المضادة للأكسدة كينازولينون وتقييم الفعالية المضادة للأكسدة

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الخلاصة

في هذه الدراسة تم تصنيع مشتقات جديدة لمركبات 1،2،4-ترايازول-كينازولينون. تم تحضير المركب الوسيط، حمض الأميك **1**، من خلال تفاعل حمض الأنثرانيليك مع كلوريد بارا ميثوكسي بنزويل. تم تحضير مركب البنزوكسازينون **2** عن طريق تفاعل حمض الأميك مع أنهيدريد الأسيتيك، وتمت الأسترة باستخدام

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هيدروكلوريد إيثيل جليسينات.حيث تم الحصول على مشتق استر **3**. تضمن المسار الأول من البحث تفاعل مشتق الإستر **3** مع (سيمي كاربازيد، ثيوسيمي كاربازيد، وفينيل ثيوسيمي كاربازيد، فينيل ثيوسيمي كاربازيد) على التوالي لإعطاء المشتقات **5**–**8**. تم حوقله المركبات **5**–**8** في وسط قلوي (2N–NaOH) وأعطى مشتقات 1، 2، 4 تريازول **9**–**12**، على التوالي. من جانب اخر، تم تفاعل المركب **4** مع CS_2 في وسط قلوي (20% KOH) لإنتاج ملح البوتاسيوم **13**. ثم تفاعل هذا المركب مباشرة مع الهيدرازين المائي لإنتاج المركب **14**. تم إثبات التركيبات الجديدة المحضرة باستخدام التقنيات الطيفية [FT–IR، 1H–NMR، C–13NMR]. الجزء الأخير من هذا البحث تم فيه اختبار هذه المواد **5**، **9**، **11**، **12**، **13**، **14** لنشاط مضادات الأكسدة باستخدام تقنية نشاط الكسح الجذري .DPPH

1. Introduction

Quinazolinones are an important class of heterocyclic compounds that exhibit a wide range of biological activities, including antimicrobial effects [1]. Specifically, quinazolinones have demonstrated potential as antimalarial [2], anticancer [3], anti-inflammatory [4], antihypertensive [5], anticonvulsant [6], and cytotoxic agents [7]. These compounds were synthesized from various precursors using different methods. The six-membered aromatic ring pyrimidine, composed of carbon and two nitrogen atoms at positions 1 and 3, is a key structural component. The body's defense systems are composed of the chemical properties of the pyrimidine nucleus, which is naturally present in nucleic acids, vitamins, coenzymes, and nucleotides, along with alkaloids produced by tea, coffee, chocolate, and uric acid.Since pyrimidine-containing compounds are essential for biological processes in pharmaceutical, agrochemical, and materials sciences[8], several synthesis techniques have been proposed. As a result, numerous synthesizin methods have been suggested. They are frequently used as medications and drug intermediaries due to their extensive range of pharmacological features, which include their capacity to act as anti-inflammatory[9], anti-microbial[10], antidiabetic[11], and anti-Alzheimer agents[12] . It is known that five-membered rings containing nitrogen atoms belong to a wide and diverse class of heterocyclic compounds that exhibit a variety of biological effects. Members of the group, including pyrazole, imidazole, oxazole, triazole, tetrazole, oxadiazole, thiazole, and isoxazole[13], have antibacterial, antifungal, and cytotoxic activity [14]. The five-membered atoms. On the other hand, triazole compounds also exhibit a wide range of actions, including anti-tumor [15], antimicrobial, anti-tubercular agents[16], anticancer [17] , and antiviral [18]. Additionally, a new class of antibacterial and antiradical compounds is represented by 1, 2, 4-triazoles. Due to the importance of 1, 2, 4-triazoles in biological processes and their ability to be synthesized, their chemistry and fused heterocyclic derivatives products garnered a lot of attention [19] .The primary objective of this research is to synthesize a new 1,2,4-triazole quinazolinone derivative and evaluate its antioxidant activity.

2. Experimental

Chemicals from Merck, BDH, Sigma Aldrich, and Fluka were utilized in this experiment without undergoing additional purification. Digital Stuart Scientific SMP3 melting point equipment and raw data were used to calculate the melting points. A SHIMAZU FTIR 8400 spectrophotometer was used to record the Fourier transform infrared (FT-IR) spectra of KBr discs in the (500-4000 cm^{-1}) spectral region. The 1HNMR and 13CNMR spectra were recorded using a Burker 400MHz apparatus with DMSO-d6 as the solvent and TMS standared.

*2.1 Synthesis of 2-(4-methoxy benzamido) benzoic acid. **1***

Anthranilic acid (1g, 0.0073 mole) was dissolved in dry acetone under stirring conditions. Subsequently, 4-methoxybenzoyl chloride (0.98 mL, 0.0073 mol) was introduced to the

solution in the presence of pyridine. The resulting mixture was heated in a water bath maintained at a temperature range of (50-60) °C for a duration of 3 hours[20]. The reaction mixture was cooled to room temperature once the heating had finished, and the solid crude was filtered, washed with water, dried, and then recrystallized from ethanol to produce the title product **1**

2.2 Synthesis 2-(4-methoxy phenyl)-4H-benzo [3, 1] oxazin- 4-one. ***2***

In dry conditions, acetic anhydride (0.008 mol) was added to compound **1** (1 g, 0.008 mol) and refluxed for 4 hours [20]. The mixture was first cooled to room temperature. Then, the reaction mixture was added to a 500 ml glass beaker containing cold petroleum ether, which caused the product to precipitate out of solution. Then solid product was washed with water and recrystallized from ethanol to obtain the indicated product **2.**

2.3 Synthesis 2-(4-methoxyphenyl)-3-ethylacetate)-quinazoline-4(3H) - one. ***3***

Ethylglycinate hydrochloride (0.5 g, 0.001 mol) was dissolved in 1 mL of dry dimethylformamide (DMF) in the presence of dry pyridine (0.5 mL) and added to a stirred solution of compound **2** (1 g, 0.0039 mol) dissolved in 3 mL of anhydrous dimethylformamide. After that, the mixture was refluxed for 4 hours, after which the resulting mixture was poured into an ice-cold solution (5% HCl) to form solid crystals that recrystallized from the ethanol into the product **3.** [21]

2.4 Synthesis 2-(4-methoxyphenyl)-3-(2-aceto hydrazide)-quinazoline-4(3H)-one. ***4***

2-(4-methoxyphenyl)-3-(2-aceto hydrazide)- quinazoline- 4(3H)-one was made through adding hydrazine hydrate 80 % (0.15 ml, 0.002 mol) to solution of compound **3** (0.5 g ,0.002mol) in 10 mL absolute ethanol, upon complete addition of the reagents, the resulting reaction mixture was stirred vigorously for 30 minutes at room temperature. Subsequently, it was heated under reflux for 8 to 10 hours, yielding a solid crystalline precipitate [21]. When the materials were kept overnight under refrigerated conditions, they were washed with a solution. distilled. Water and its recrystallization from acetone to product **4.**

2.5 Synthesis 2-(4-methoxyphenyl)-3-amino aceto semicarbazide ***5****; thiosemicarbazide* ***6****; phenylsemicarbazide* ***7****; phenylthiosemicarbazide* ***8*** *-quinazoline-4(3H) - one.*

0.5 g (0.002 mol) of compound 3 was dissolved in 7 ml of ethanol. A few drops of DMF were added to the solution. This mixture was then added separately to 0.002 mol each of semicarbazide, thiosemicarbazide, phenylsemicarbazide, and phenylthiosemicarbazide. 0.15 g (0.002 mol) of sodium acetate was then added to each reaction mixture. The mixtures were refluxed for 18-20 hours. After cooling, the reaction mixture was placed in ice water to precipitate. After filtration, the precipitate is recrystallized using a suitable solvent to obtain the desired products **5-8**. respectively [22]

2.6 Synthesis 2-(4-methoxyphenyl)-3-(5-hydroxy -4-H-1,2,4-triazol-3-yl) ***9****; 5-mercapto -4H - 1,2,4-triazol-3-yl* ***10****; 5-hydroxy -4-phenyl-1,2,4- triazol -3- yl* ***11****; 5-mercapto-4-phenyl-1,2, 4-triazol-3-yl [12] –quinazoline-4(3H)-one.* ***12****.*

Mix (0 .0 0 1 mol) of one of compounds **5-8** with 2N aqueous NaOH solution (20 ml) and reflux the mixture for 12 to 14 hours. Cool the mixture to room temperature, immerse it in ice water. Neutralize the mixture using hydrochloric acid (1:1), the precipitate formed is filtered, and the precipitate is recrystallized using a suitable solvent to obtain the desired products.**9-11**. with a suitable solvent [22]

*2.7 Synthesis of 2-(4-methoxyphenyl) -3-(aminoaceto dithiocarbazide) -quinazoline-4(3H) -one. **13***

To a stirred solution of the hydrazide derivative **4** (0.5 g, 0.0022 mol), a solution of potassium hydroxide (0.12 g, 0.0022 mol) in absolute ethanol (15 mL) was added dropwise. Subsequently, carbon disulfide (0.13 g, 0.0022 mol) was introduced slowly to the mixture, which was then stirred overnight .Then (15 ml) dry ether is added to the mixture.[22] A precipitate is obtained. It is filtered, washed with ether, dried, and can be used in the second stage to obtain compound **13.**

*2.8 2-(4-methoxyphenyl) - 3-((4-amino-5-mercapto-4H-1, 2, 4-triazol-3-yl) methyl)-quinazolin-4(3H)-one. **14***

A solution of potassium salt **13** (0.4 g; 0.0011 mol) is refluxed in excess hydrazine hydrate (4 mL) until hydrogen sulfide production ceases. We notice that the color of the reaction mixture turns yellow during reflux.[22] After cooling, the mixture is acidified by adding 10% HCl to the reaction liquid, producing a yellow precipitate. The crystals were produced by recrystallizing the precipitate made from ethanol to obtain the desired product **14**.

2.9 Anti-oxidant activity

The antioxidant activity of each sample was assessed using the DPPH (2,2-diphenyl-1-picrylhydrazyl) free radical scavenging method. Each sample was dissolved in 5 mL of dimethylformamide (DMSO) to prepare a 200 ppm stock solution, by dissolving 1 mg of the sample in the solvent. Then, prepare a concentration of 150 ppm by dissolving 1.5 mL of the solution in 1 mL of DMSO. You can also prepare a concentration of 100 ppm by dissolving 1 mL of the solution in 1 mL of DMSO.[23] Finally, prepare the 50 ppm concentration by dissolving 0.5 ml of stock solution in 1.5 ml of DMSO. To measure the effectiveness, three concentrations were created from each sample. One mL of each concentration was then added to one mL of a 50 ppm DPPH solution in a test tube, and the samples were then placed in an incubator for 30 minutes without exposure to light. The efficacy was then measured using a spectrophotometer at a wavelength of 517 nm and compared to a standard ascorbic acid solution. Table 3 shows the results of calculating the IC_{50} for samples after combining 1 mL of methanol with 1 mL of DPPH solution 50 ppm dissolved in DMSO to create the blank solution.

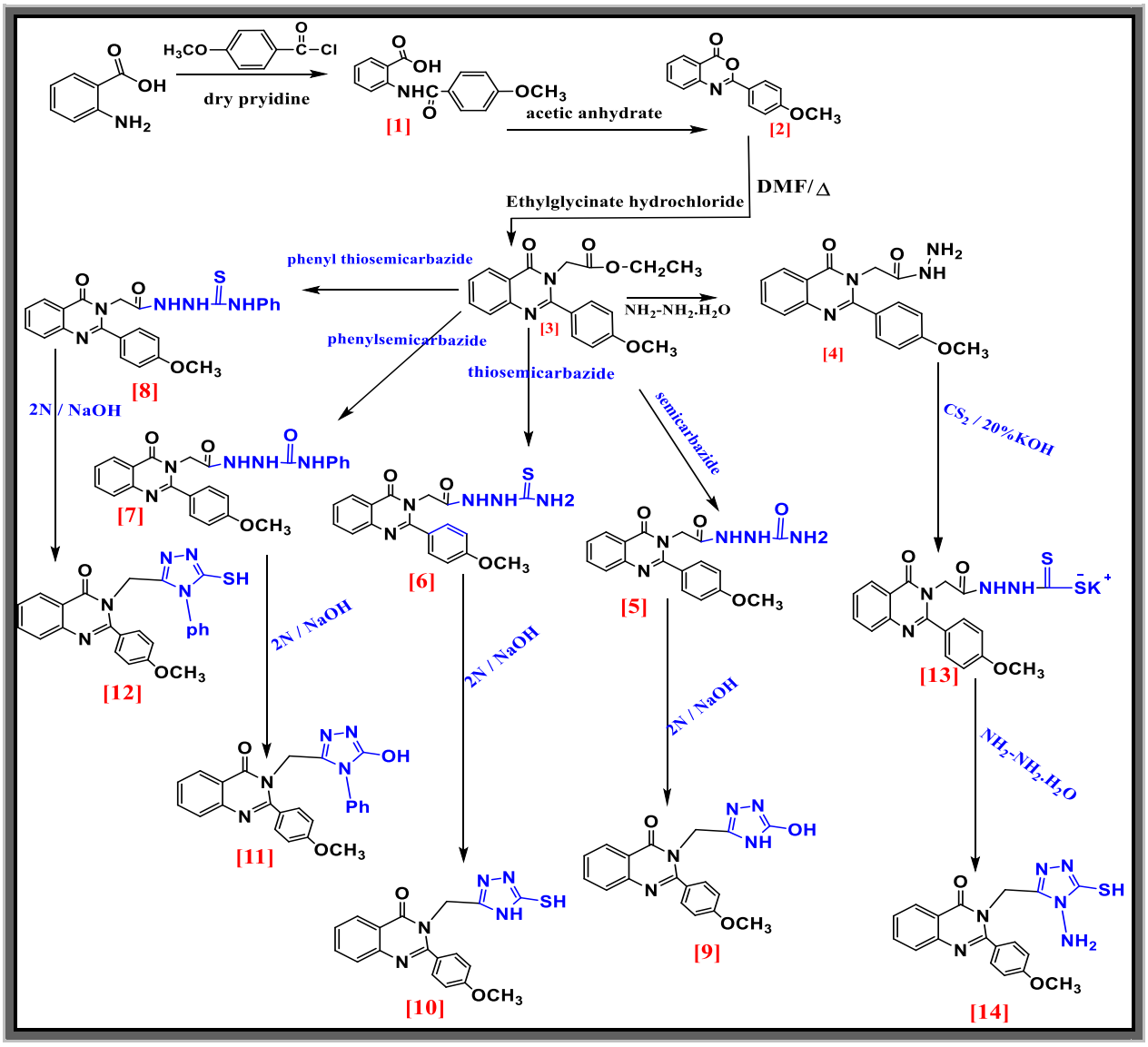
3. Result and Discussion

The primary objective of this research was to synthesize novel target compounds, as depicted in Scheme 1. In the first step, compound **1** was prepared by reacting anthranilic acid with 4-methoxybenzoyl chloride, using pyridine as a catalyst. Dry acetone was used as a solvent for 3 hours, and so on, in the second step, compound **1** reacts with acetic anhydride in an annular closure reaction to give benzoxazinone **2**. In the third step, compound **2** reacted with ethylglycinate hydrochloride, provided that the intermediate is basic and the solvent used for this reaction is dry Dimethylformamide, where pyridine and sodium hydroxide are used to prepare the basic starting material. We followed these steps to prepare compound **3**, which was treated with an excess amount of hydrazine hydrate to produce compound **4**. The physical properties of compounds **1-4** are shown in (Table1).

The FTIR spectrum of compound **1** showed absorption bands at 3257 cm^{-1} corresponding to N-H stretching, 3068 cm-1 attributed to the aromatic C-H stretch, and 1710 cm-1 assignable to the C=O stretch of the acid. The amide acid was observed at 1672 cm^{-1}. A broad absorption in the range of 3448-2700 cm-1 corresponded to the O-H stretch and is listed in Table 1. The FTIR spectrum data of compound **2** shows the absorption band of the lactone v(C=O) at (1760 cm^{-1}). The FTIR spectrum data of compound **3** show that the absorption

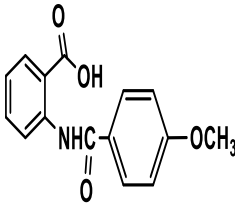
band at 1760 cm^{-1} disappeared for the ν lactone (C=O), and a new absorption band appeared at 1747cm^{-1} for the ν ester (C=O). The FTIR spectroscopic data for compound **3** are listed in (Table1). While the 1H-NMR spectroscopic data show a triplet signal at δ = 1.32 ppm belonging to the 3H of (-CH_3), the quadruple signal at δ = 4.35 ppm belongs to the 2H of (-OCH_2), the single signal at δ = 3.85 ppm belongs to the 2H of (O-CH_3), the single signal at δ = 5.08 ppm belongs to the 2H of (N-CH_2) and the multiple signal at δ = 7.09-8.66 It belongs to 8H (Ar-H). The 1H-NMR and 13CNMR spectral data for compound **3** are shown in (Table 2). The FTIR spectrum data for compound **4** show that the ν(C=O) absorption band of the ester has disappeared and a new band 1668 cm^{-1} appeared in its place, two bands at 3436 and 3290 cm^{-1} also appear to belong to the asymmetric υ(-NH_2) and symmetric respectively. The FTIR spectroscopic data for compound **4** are listed in (Table.1). Semicarbazide derivatives were prepared by reacting compound **3** with (semicarbazide **5**, thiosemicarbazide **6**, phenylthiosemicarbazide **7**, and phenylthiosemicarbazide **8**) respectively as shown in (Scheme 1).

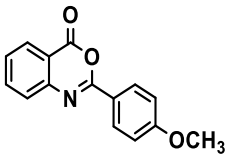
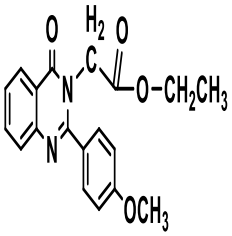
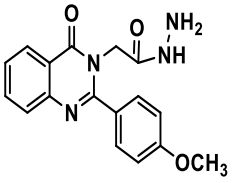
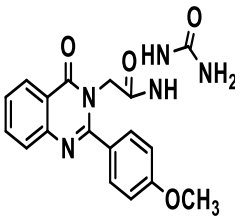
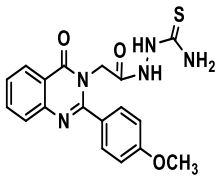
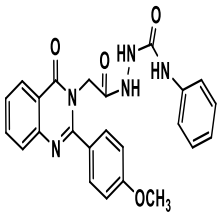
The FTIR spectroscopic data showed absorption at (3326-3336) cm^{-1} asymmetric of ν(-NH_2), and symmetric of ν(-NH_2) at (3284, 3211) cm^{-1} respectively of compound **5** and **6**, (3298-3153) cm^{-1} for ν(-NH) also absorption bands at (1683-1672) cm^{-1} for ν(C=O) amide , while the data of 1H-NMR and 13 CNMR spectra in DMSO-d6 solvent for Compound **6** all signal shown in table 2 , that contain of signal in 3.85 (s, 3H, -O-CH_3), 4.11(s, 2H,-N-CH_2), 7.07-8.65(m, 8H, Ar-H), 7.90(s,1H,-NNH) ,8.67(s, 1H, O=C-NH) and 9.55(s, 2H, -NH_2) .13C-NMR spectrum data of this compound **5-8** were listed in (Table.2) . Treatment of compounds **5-8** with (2N. NaOH) solution afford intramolecular cyclization to give the hydroxytriazole **9**, thiotriazole **10** phenylhydroxytriazole **11** and phenylthiotriazole **12** and were identified from FTIR spectra shows result in (Table.1). All the spectrum data showed the presence of absorption of ν(-NH) (3232 and 3211) cm^{-1}, absorption bands of ν(C-H) Aliph at (2979-2839) cm^{-1}, absorption bands of ν(C=O) of at (1681-1666) cm^{-1}, and absorption bands of imine groups ν(C=N) group at (1650-1639) cm^{-1} of compound **9-12**. The compound **9-12** have ν (OH) group at (3429-3402) $cm^{-1.}$ While the 1H-NMR spectra data in DMSO-d6 solvent of compound **9-12** show in (Table 2) the signal of compound **10** was 3.51(s,3H, -O-CH_3), 4.57(s,2H, NCH_2), 7.13-8.64(m,8H, Ar-H) ,11.28(s,1H, NH) ,12.55(s,1H, -SH), While the compound **11** show signal in 3.51(s,3H, -O-CH_3), 4.57(s,2H, -N-CH_2),7.03-8.54(m,8H, Ar-H), and 12.08(s,1H, OH).

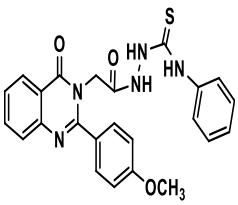
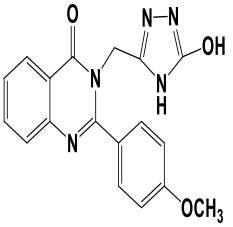
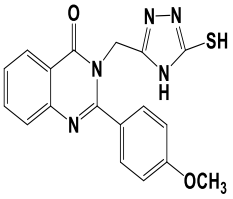
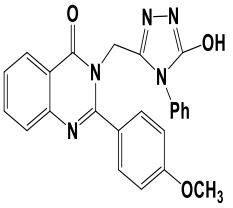
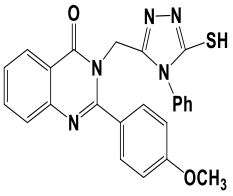
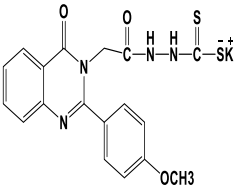
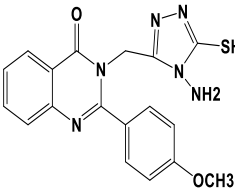


Scheme 1: Synthesis of new novel 1, 2, 4-triazole derivatives bearing 3(4H)-quinazolinon ring **(1-14)**

Table 1: Physical characteristics and FT-IR data spectra of all novel synthesized compounds **(1 – 14).**

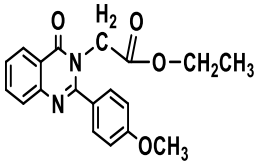
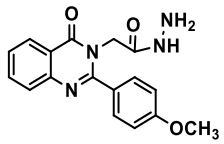
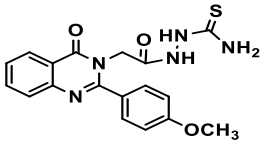
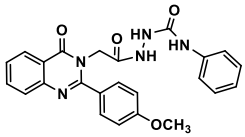
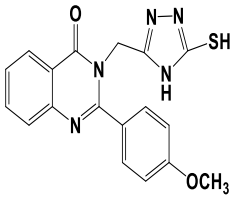
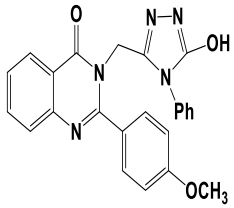
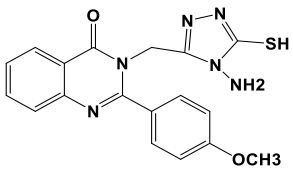
No	Structure	Molecular Formula	M.P. C ⁰	Color	Yield (%)	solvent for purification	FT-IR(νcm^{-1})
1		$C_{15}H_{13}NO_4$	212-214 °	Pale yellow	90	Ethanol	3448-2700 ν (O–H), 3257 ν(NH),3068 ν(Ar-H),2974, 2929 ν (CH aliph), 1710 ν (C=O acid),1672 ν (C=O amide), I604,1591 ν(C=C),1203,1176 ν(C-O-C), 776 ν (p-position)

2		$C_{15}H_{11}NO_3$	158-160	white	90	Ethanol	3028 ν(Ar-H), 2952,2837 ν (CH aliph), 1760 ν (C=O lactone), 1641ν (C=N), 1602,1568ν (C=C), 1218,1168ν(C-O-C) 773 ν (p-position)
3		$C_{19}H_{18}N_2O_4$	99-100	Light Orang	80	Ethanol	3072ν (Ar-H), 2977, 2937 ν(CH-aliph), 1747 ν(C=O) ester, 1668, ν(C=O) quinaz., 1641 ν(C=N), 1606,1571 ν(C=C), 1213,1182 ν(C-O-C), 757ν (p-position)
4		$C_{17}H_{16}N_4O_3$	180-182° C	White	75	Acetone	3436 Asym,3290 sym ν(NH_2), 3182 ν(NH), 3002 ν(Ar-H), 2977,2939 ν (CH aliph), 1668 overlap ν(C=O) amide with (C=Oquinaz.), 1579 ν(C=C)
5		$C_{18}H_{17}N_5O_4$	166-168 °C	Yellow	92	Dioxane	3326 asym, 3284 sym ν(NH2), 3203 ν(NH), 3074 ν (Ar-H), 2985,2839 ν (CH aliph), 1693 ν (C=O quinaz), 1672 ν (O=C-NH2), 1649 (C=O amid), 1596 ν(C=C),1253,1180 ν(C-O-C), 846 ν (p-position)
6		$C_{18}H_{17}N_5O_3S$	190-192 °C	deep yellow	83	Dioxane	3336 asym,3211 sym ν(NH2), 3153 ν(NH),3070 ν (Ar-H), 2972, 2839 ν (CH aliph), 1683 ν(C=O) quinaz,1652ν (C=O amid),1604 (C=C), 1404(C=S), 1249,1178 ν(C-O-C), 840 ν (p-position)
7		$C_{24}H_{20}N_5O_4$	198-200	Purple	75	Dioxane	3296 ν(NH), 3076 ν (Ar-H), 2979,2840 (CH aliph), 1710(C=O quinaz), 1683(O=C-NHPh), 1666(C=O amid), 1593ν (C=C), 1253,1178 (C-O-C) ,823 ν (p-position)

8		$C_{24}H_{21}N_5O_3S$	145-147	Pale brawn	70	Dioxane	3284ν(NH), 3026 ν (Ar-H),2970,2844 ν (CH aliphatic), 1689 ν (C=O quinaz),1670 (C=Oamid) ,1606(C=C), 1413(C=S),1251,1190 ν(C-O-C),846 ν (p-position)
9		$C_{18}H_{15}N_5O_3$	194-196	white	80	Ethanol	3402 ν (OH), 3232 ν(NH) ,3072 ν (Ar-H), 2975,2840 ν (CH aliph) ,1660 ν (C=O quinaz), 1643 (C=N), 1604,1585 ν (C=C), 1253,1182ν (C-O-C), 840ν (p-position)
10		$C_{18}H_{15}N_5O_2S$	225-227	Pale yellow	75	Ethanol	3211ν(NH),3051ν(Ar-H),2975 ,2839 ν (CH aliphatic), 2585 ν(SH), 1679 (C=O quinaz.), 1641 (C=N), 1573 ν(C=C), 1255,1178 ν(C-O-C), 848 ν (p-position)
11		$C_{24}H_{19}N_5O_3$	160-162	Pale pink	85	Ethanol	3429 (OH), 3068(Ar-H), 2974, 2842(CH aliph), 1666, (C=O quinaz.),1639(C=N) ,1602, 1568 (C=C), 1253,1180, (C-O-C) , 837 ν (p-position)
12		$C_{24}H_{19}N_5O_2S$	125-127	Light green	80	Ethanol	3095, 3055(Ar-H), 2977, 2839(CH aliph), 2557(SH), 1681 (C=O quinaz),1650(C=N), 2557 ν (SH), 1251,1178 ν(C-O-C),781 ν (p-position)
13		$C_{18}H_{15}KN_4O_3S_2$	233-235	yellow	90	Ether	3257(NH),3064(Ar-H),2935,2839 (CH aliph),1674 (C=O quinaz), 1645(C=O amide) ,1604 (C=C), ν(C=S) 1369, 1255,1178 ν (C-O-C), 838 ν (p-position)
14		$C_{18}H_{16}N_6O_2S$	197-199	light brown	75	Ethanol	3458asym,3396sym ν(NH_2), 3058 ν(Ar-H), 2977 ,2835 ν(CH aliph), ν (SH) 2559 .1681 (C=Oquinaz),1647(C=N) triazole, 1587,1562 (C=C), 1257,1176(C-O-C) ,840 ν (p-position)

Ultimately, for the synthesis of compound **14**, the reaction of compound **4** with carbon disulfide (CS2) in ethanolic potassium hydroxide (KOH) yielded the dithiocarbazate salt **13** in excellent yield. This salt **13** was subsequently cyclized by refluxing with 80% hydrazine hydrate, leading to the formation of the triazole derivative **14** in a very good yield. FTIR spectrum showed absorptions at (3458 cm^{-1}) asymmetrical, and (3396cm^{-1}) symmetrical for $-NH_2$ group, (1681 cm^{-1}) for (C=O quinazoline) and 1647 cm^{-1} for ν (C=N triazole) group and 2559 for SH. 1HNMR spectrum showed singlet signal at 3.51(s, 3H, $-O-CH_3$), 4.57(s, 2H, $-N-CH_2$), 5.72(s,2H, $-NH_2$) 7.13-8.64(m, 8H, Ar-H); and 12.08(s, 1H, SH), all data of 13C-NMR spectrum of this compound **3,4,6,7,10,11 and 14** were listed in table 2. [24]

Table 2: 1H-NMR and 13 C-NMR spectra data (ƍ ppm) of compounds (3-14)

Comp.No		^{1}HNMR(δppm)	13CNMR(δppm)
3		1.32(t,3H, CH_3), 3.85 (s,3H, -OCH3), 4.35 (q ,2H, O-CH_2); 5.08 (s,2H, N-CH2); 7.09-8.66(m,8H, Ar-H)	14.52(-CH_3), 41.48(N-CH_2) 55.95(-OCH_3), 61.87(O-CH_2), 114.6-147.07(Ar-C) 156.44.67(C=N), 165.82 (C=O quinaz), 170.6 (C=O ester)
4		3.85(s,3H OCH_3); 4.15(s,2H, N-CH_2), 4.67(s,2H, NH_2); 7.09-8.13(m,8H, Ar-H) 8.67(s,1H,NH)	41.8(N-CH_2), 55.95(-OCH_3); 113.21-148.46 (Ar-C); 164.45 (C=O quinaz) ,168.82 (C=O amid)
6		3.85(s,3H, O-CH_3) 4.11(s,2H, -N-CH_2); 7.07-8.65(m,8H, Ar-H); 7.90 (s, 1H, NNH) 8.67(s,1H, O=C-NH) 9.55(s,2H, NH_2)	47.82(N-CH_2), 55.04(-OCH_3) 114.67-147.07 (Ar-C); 165.82 (C=O quinaz); 169.74 (C=O amid); 191.43(C=S)
7		3.78(s,3H, O-CH_3) 4.64(s,2H, -N-CH_2), 7.13-8.64(m,12H, Ar-H); 8.74(s,1H, NH-Ph) 9.12(s,1H, -C=O-NH), 9.8 (s,1H,-NHNH)	47.82(N-CH_2), 55.96(-OCH_3) 114.67-147.07(Ar-C), 162.80(C=O-Ph), 165.82 (C=Oquinaz) 169.74 (C=O amid)
10		3.51(s,3H, Ph-O-CH3),4.57(s,2H, -N-CH2), 7.13-8.64(m,8H, Ar-H); 11.28(s,1H,-NH),12.55(s,1H,-SH),	41.50(N-CH_2),56.11(-OCH_3), 114.67-147.07 (Ar-C) ,156.50, 162.69 (C=N triazole ring),165.82 (C=O quinaz)
11		3.51(s,3H, Ph-O-CH3) 4.57(s,2H, -N-CH2), 7.03-8.54(m,8H, Ar-H); 12.08(s,1H,-OH)	45.90(N-CH2),55.31(-OCH3), 114.67-147.07 (Ar-C) 148.47.50,162.75, (C=N triazole ring),165.82 (C=O quinaz)
14		3.51(s,3H, O-CH3) 4.57(s,2H, -N-CH2), 5.72(s, 2H, NH_2) 7.13-8.64(m,8H, Ar-H); 12.08(s,1H,SH)	47.07(N-CH2),55.92(-OCH3), 114.67-147.07 (Ar-C), 156.50,162.96 (C=N triazole ring),165.82 (C=O quinaz),

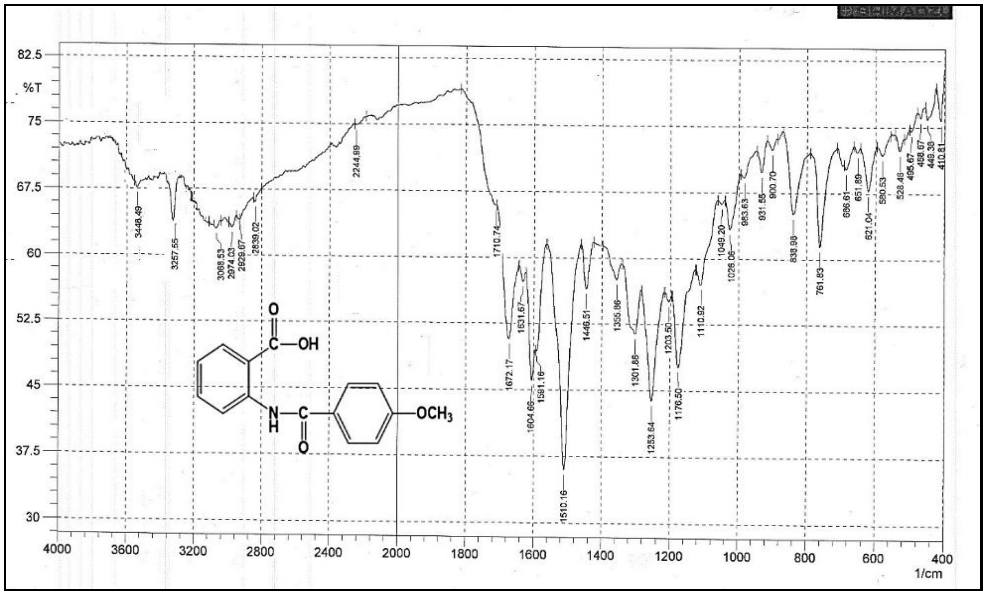


Figure1: FT-IR spectra of compound (1)

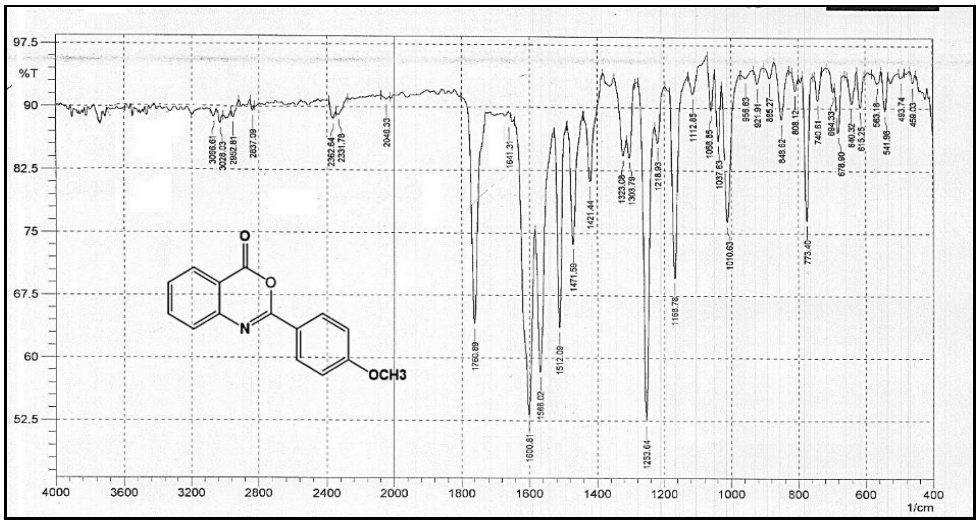


Figure2: FT-IR spectra of compound (2)

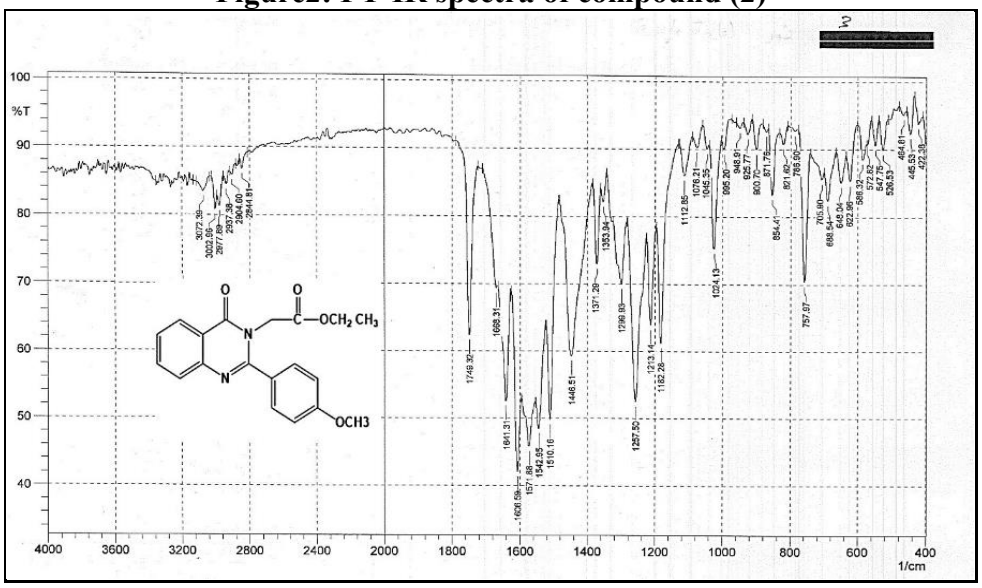


Figure3: FT-IR spectra of compound (3)

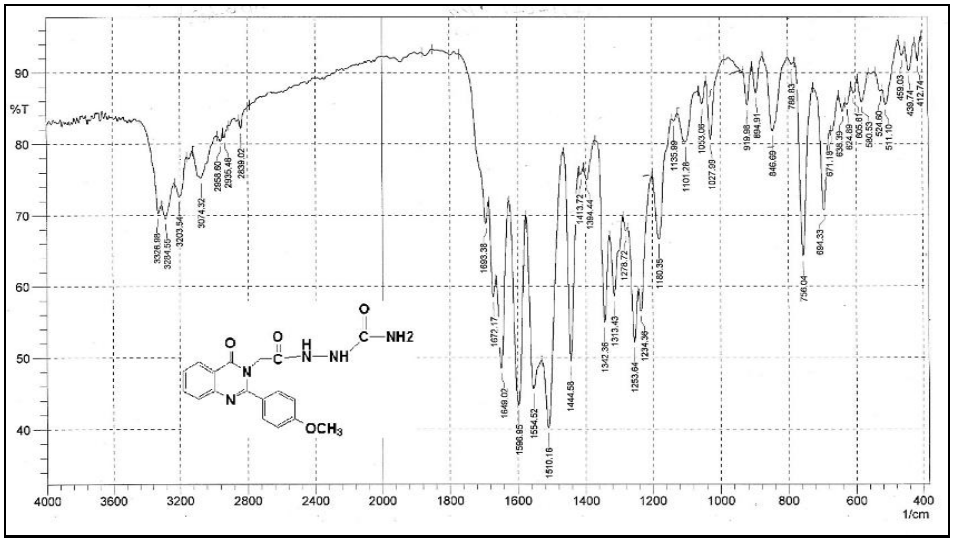


Figure 4: FTIR spectra of compound (5)

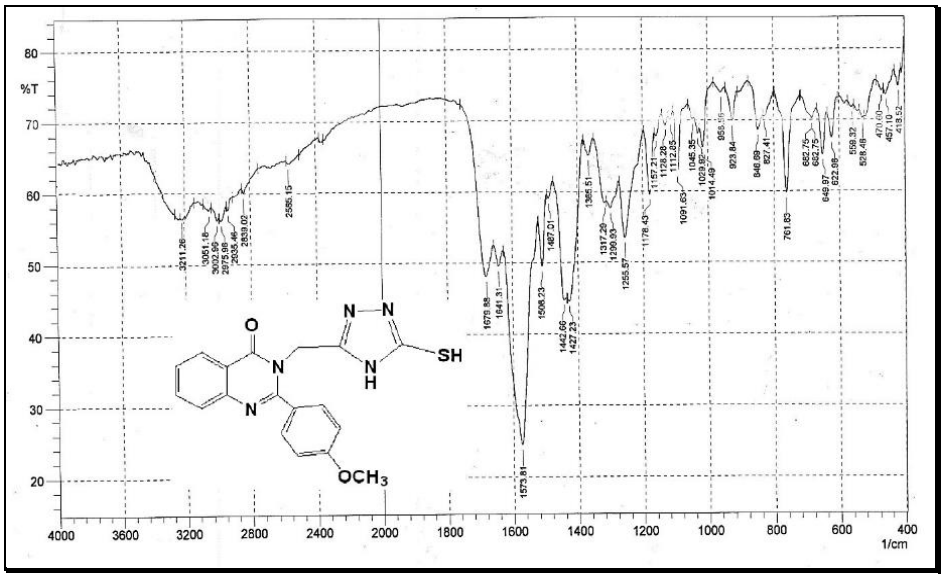


Figure 5: FTIR spectra of compound (10)

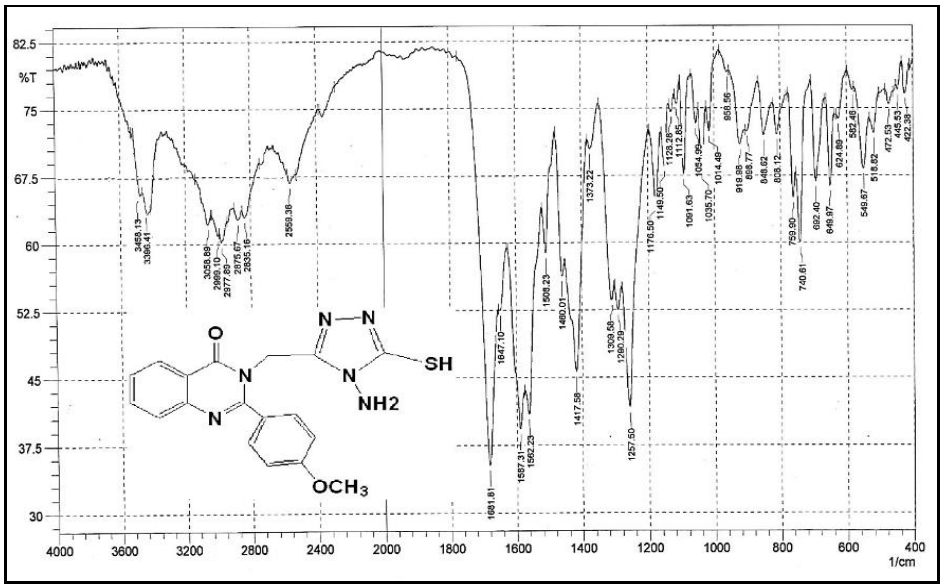


Figure 6: FT-IR spectra of compound (14)

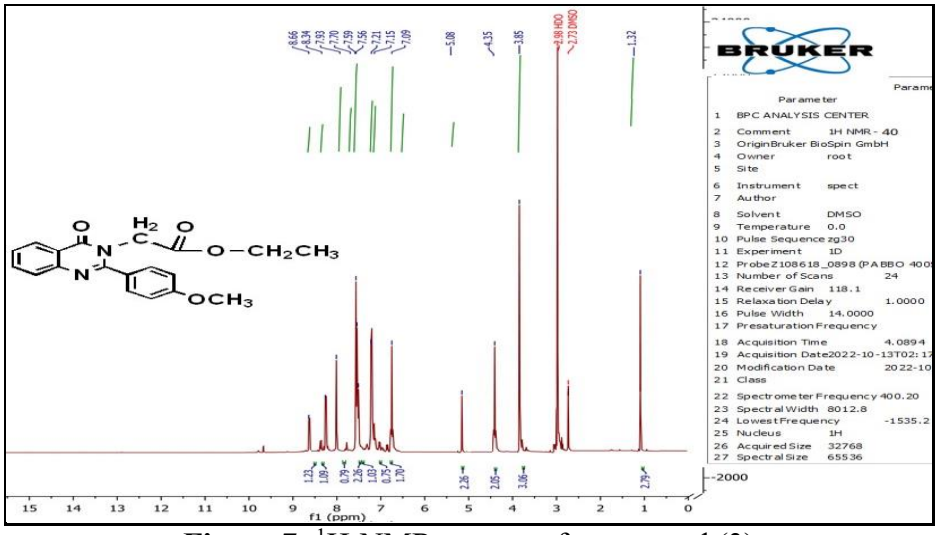


Figure 7: [1]H-NMR spectra of compound (3)

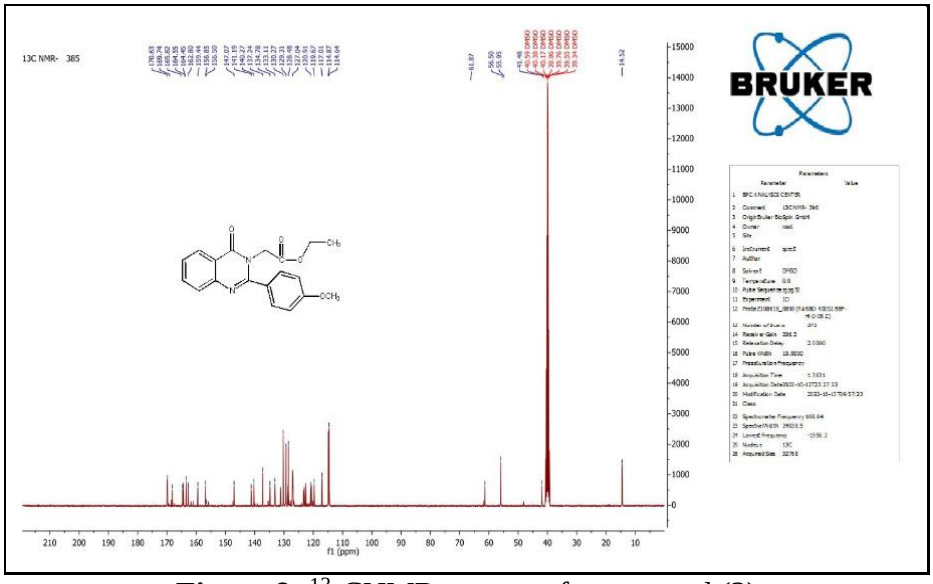


Figure 8: [13]-CNMR spectra of compound (3)

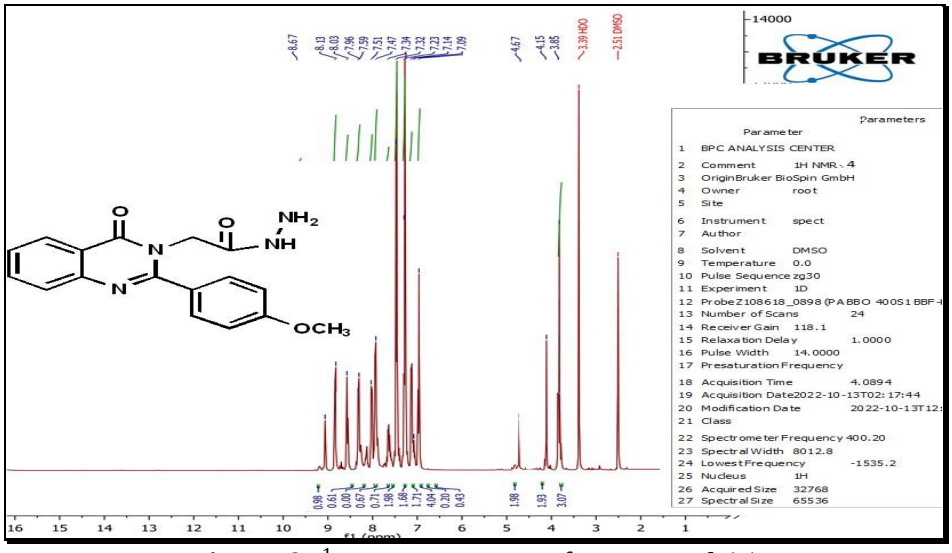


Figure 9: [1]H-NMR spectra of compound **(4)**

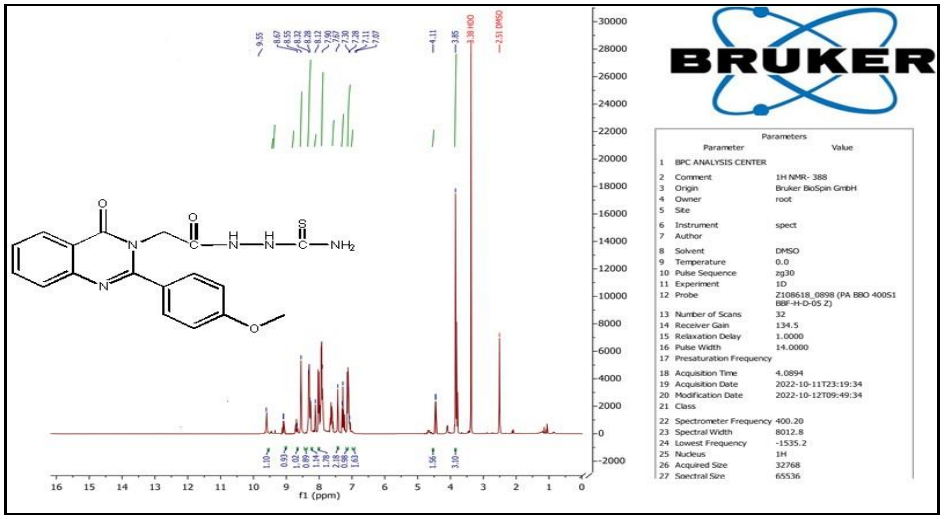


Figure 10: 1-HNMR spectra of compound (6)

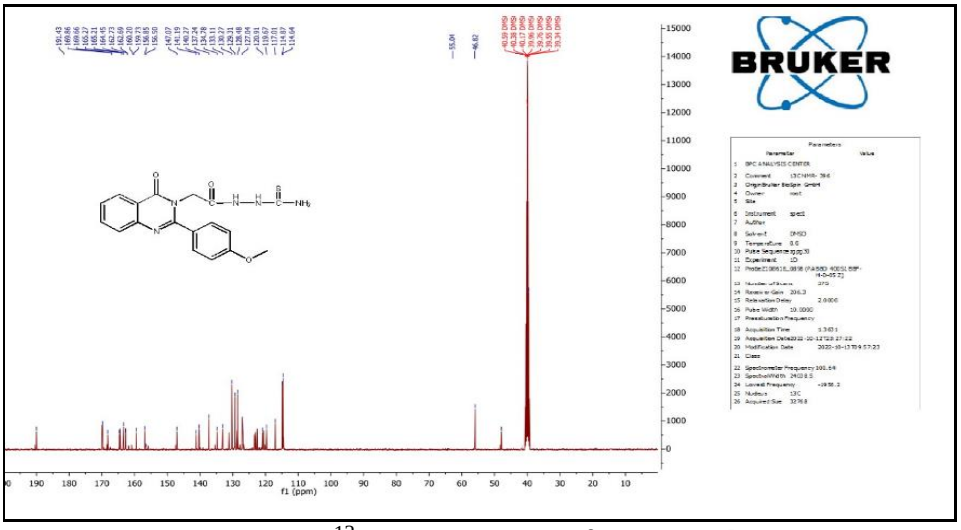


Figure 11: ^{13}-CNMR spectra of compound (6)

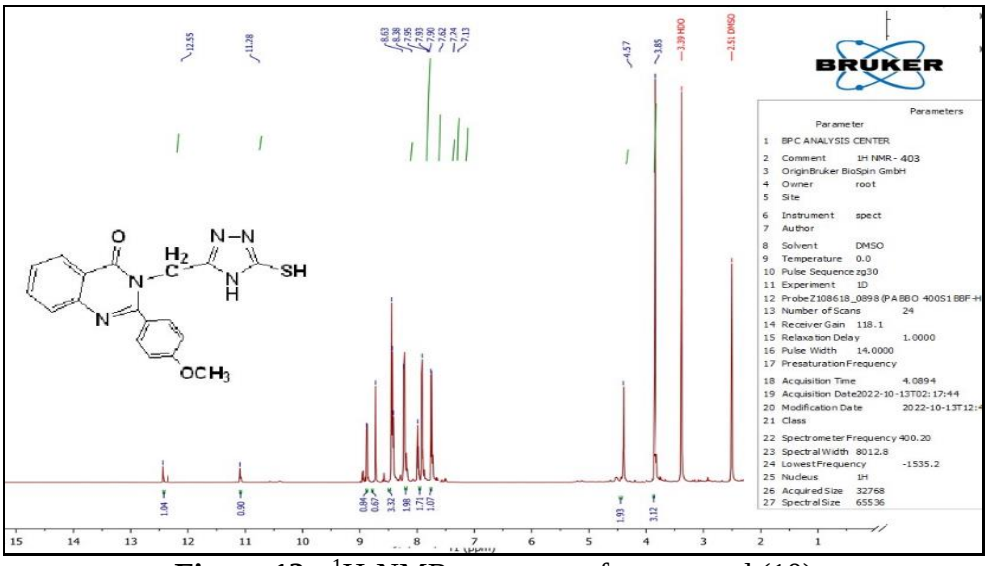


Figure 12: ^{1}H-NMR spectrum of compound (10)

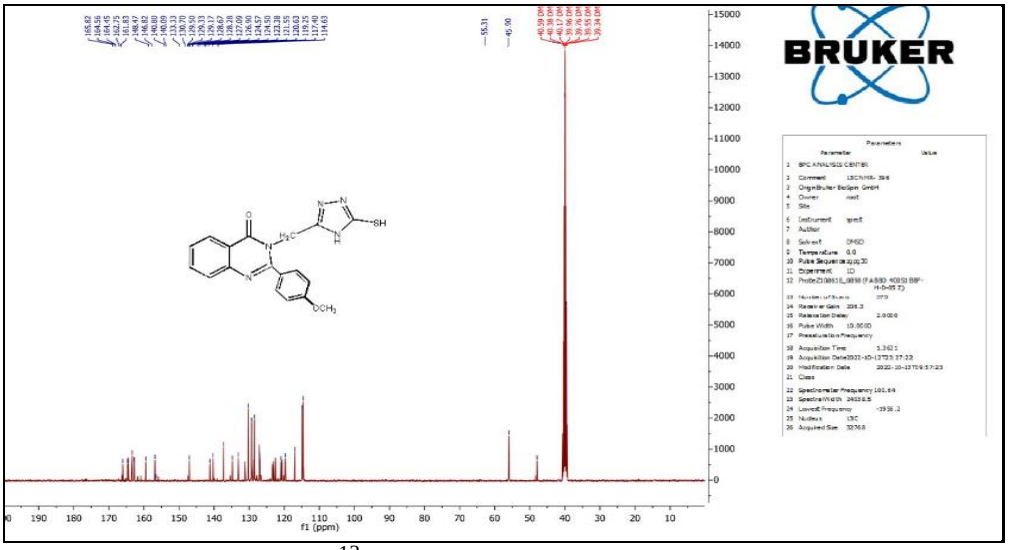


Figure `13: ^{13}C-NMR spectrum of compound (10)

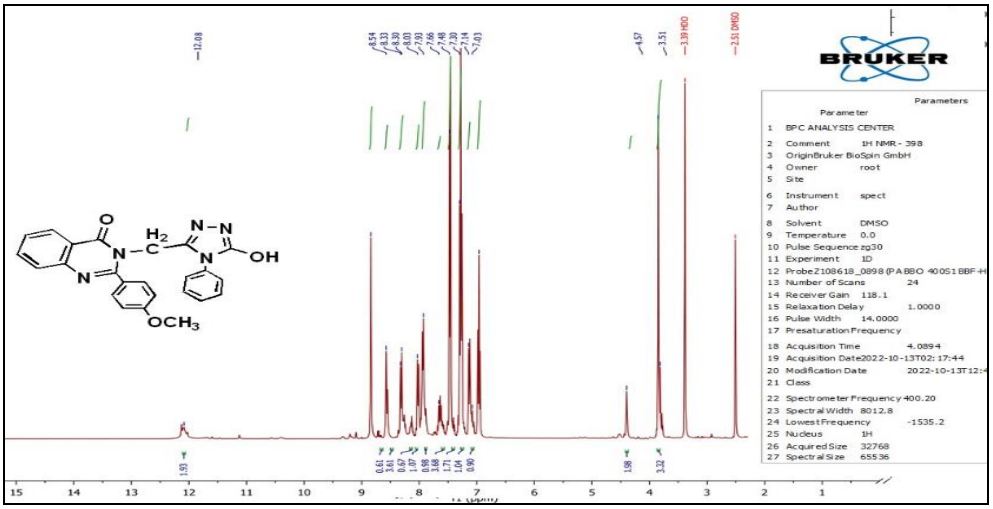


Figure 14: ^{1}H-NMR spectrum of compound (11)

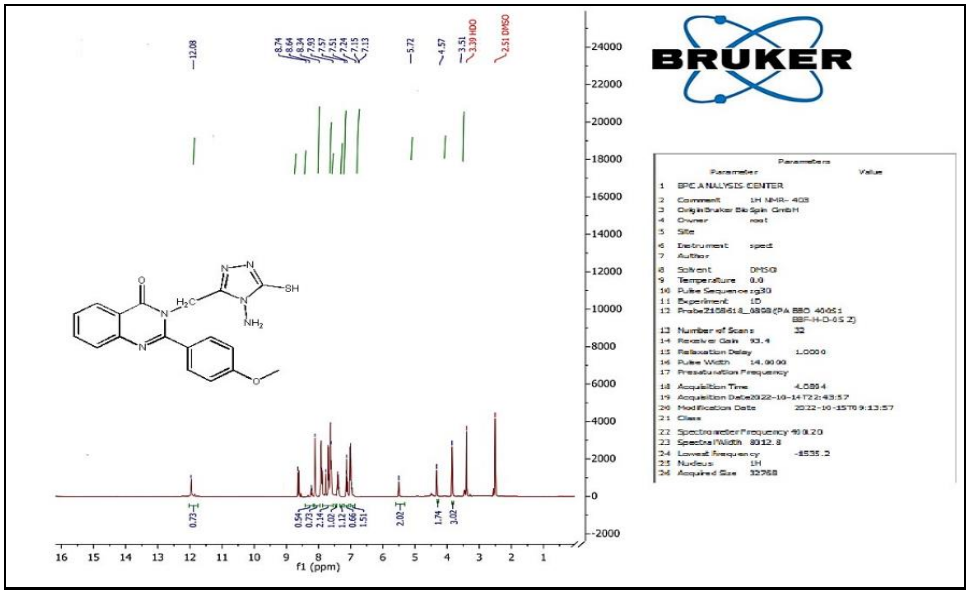


Figure 15: ^{1}H-NMR spectrum of compound (14)

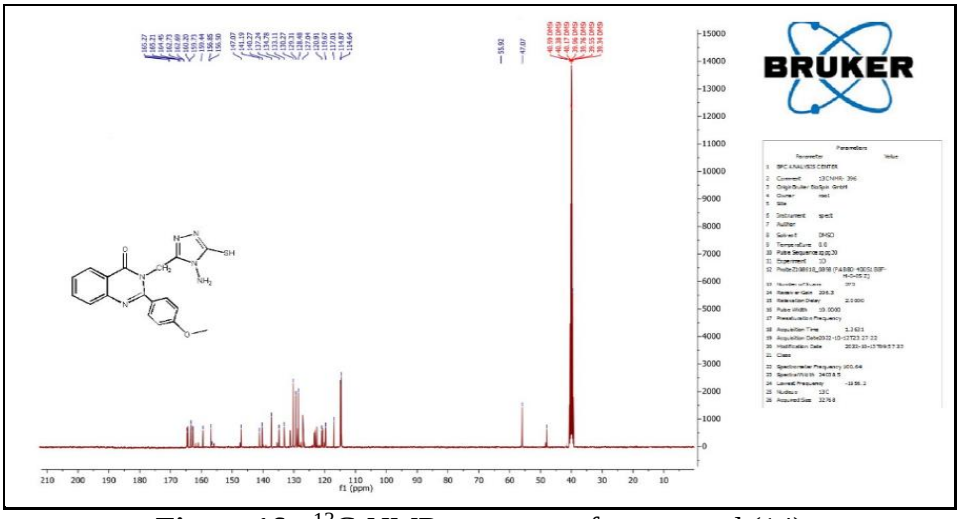


Figure 16: ^{13}C-NMR spectrum of compound (14)

3.1 Anti-Oxidant Activity

Antioxidants possess potent free radical scavenging capabilities, effectively slowing down or preventing the oxidation of easily oxidizable compounds within living organisms. These antioxidant substances play a crucial role in protecting cells and macromolecules from the damaging effects of free radicals [25]. The search for antioxidant compounds has taken on increasing importance in recent years [26]. Synthetic antioxidants are being utilized more frequently than natural antioxidants since they are less expensive and more powerful. It was calculated using the test method DPPH at various concentrations (50, 100, 150, and 200 µg/ml) [27]. With concerning the number of electrons collected, the outcome depends on the reaction that distinguishes by changing its deep violet hue (DPPH) or color fading. By referring to Table (3) and Figure (17), which present the values of antioxidant activity inhibition and the corresponding IC_{50} values, it can be observed that the highest antioxidant activity values correspond to the lowest IC_{50} values [28]. When comparing the antioxidant activity of compounds with ascorbic, we found that compounds **12, 13**, and **14** have activity similar to ascorbic, and **5, 9**, and **11** have weak activity with it.

Table3: IC50 and percentage of products that inhibit various prepared compounds 5, 9, 11, 12,13 & 14

com	conc µ/mL	RSA %	Ascorbic acid	IC_{50}	R^2	com	conc µg/mL	RSA %	Ascorbic acid	IC_{50}	R^2
5	50	26.04	75.92	2.17283	0.9832	**12**	50	55.07	75.92	1.959294	0.9752
	100	37.53	87.97				100	70.23	87.97		
	150	56.66	93.03				150	85.9	93.03		
	200	69.75	98.88				200	90.54	98.88		
9	50	33.08	75.92	3.84730	0.8775	**13**	50	74.97	75.92	2.180143	0.7204
	100	36.91	87.97				100	88.74	87.97		
	150	56.17	93.03				150	91.26	93.03		
	200	68.14	98.88				200	93.66	98.88		
11	50	26.04	75.92	1.65929	0.9752	**14**	50	77.23	75.92	2.185688	0.7726
	100	40.7	87.97				100	87.23	87.97		
	150	45.06	93.03				150	92.28	93.03		
	200	50.74	98.88				200	98.65	98.88		
Ascorbic acid	50	75.92	2.016294		0.6979						
	100	87.97									
	150	93.03									
	200	98.88									

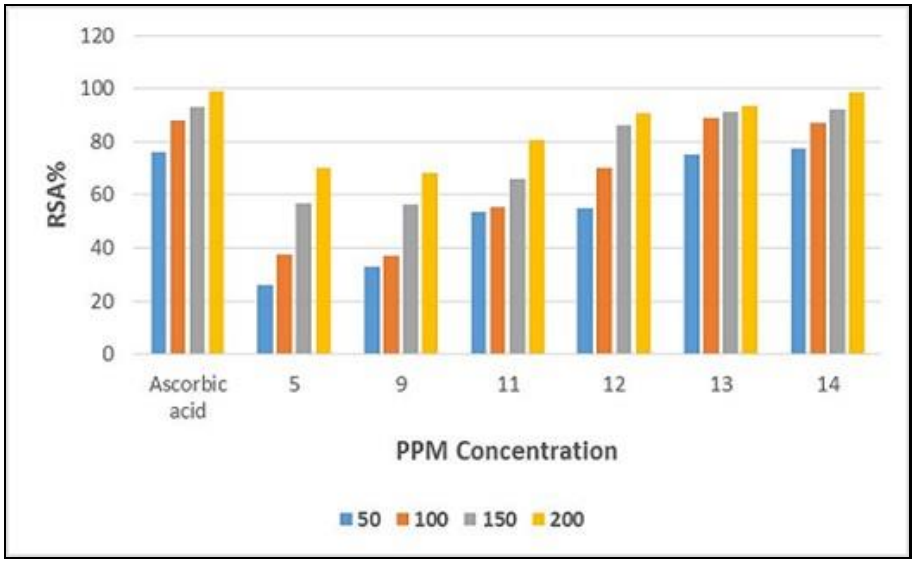


Figure 17: shows the newly synthesized compound's 5-14 capacity to scavenge DPPH

Conclusion

In this study, a series of novel 1,2,4-triazole derivatives 9-14 were synthesized with yields ranging from 70 to 90%. The structure elucidation of these 1,2,4-triazole derivatives was supported by FT-IR, 1H-NMR and 13C-NMR spectral data. The final part of this research involved evaluating the antioxidant activity of these compounds through their ability to inhibit radical scavenging. These compounds **5, 9, 11, 12, 13 &14** were examined for antioxidant activity using DPPH radical scavenging activity technology. We examined the ability of some compounds to inhibit radical scavenging with biological antioxidant activity. When comparing the antioxidant activity of tested compounds with ascorbic, we found that compounds **12, 13**, and **14** have activity similar to ascorbic, while the compounds **5, 9**, and **11** have weak activity with it.

5. Acknowledgements

The authors of this study would like to express their gratitude to the Department of Chemistry, College of Sciences, University of Baghdad, for providing materials and guidance.

6. Conflict of Interest

The authors declare that they have no any conflict of interest.

7. Compliance with ethical standards

This section states that none of the authors have examined animals or people.

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