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Synthesis and Identification of New imidazolidine-4-one Derivatives and Study of their Biological Activity as Anti-bacteria, Fungi and oxidant.

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ABSTRACT

In this study, a new heterocyclic compound called imidazolidine-4-one derivatives was synthesized by first reacting thiosemicarbazide with carbon disulfide to create gate thiadiazole compound (A). This compound then interacted with 2-hydroxy benzoic acid to create azo compound (B), which then interacted with substituted phenyl amines to create Schiff base (S_1-S_8), which then reacted with 2-amino acetic acid to produce imidazolin-4-one derivatives. These compounds are characterized by ^{1}H MNR, ^{13}C NMR, and Fourier-transform infrared spectroscopy (FT-IR). Next, we examine the biological characteristics of all heterocyclic derivatives to protect against two types of bacteria, one kind of fungus, and antioxidants. The novel-produced compounds'antioxidant activity was assessed using the DPPH. Compound G_4 (88%) have DPPH radical scavenging properties that are especially potent and equivalent to ascorbic acid. The synthesized compounds' antifungal efficacy using the diffusion method. Imidazolin-4-one derivatives were found to be more effective against Candida in an antifungal. The reducing abilities of the investigated compounds were measured. In antibacterial and anti fungi used less concentration that occur inhibition 2.5 mg/mL and high concentration used 20 mg/mL. This study provides key molecular insights that can be utilized to assess the antibacterial and antifungal activities of the Imidazolin-4-one ring and enhance its antioxidant properties.

Keywords: Azo, Imidazolidine-4-one derivatives, Schiff bases, Anti-oxidant, Anti-fungal, antibacterial

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INTRODUCTION

Schiff base has been recognized as a crucial core component in medication creation over time. The preparation of Schiff base, named for Hugo Schiff [1], involved a condensation reaction between an aldehydic/ketonic carbonyl and amino functionality [2]. Schiff bases have been shown to have a wide range of pharmacological properties, including antimicrobial [3], anticancer [4], antitumor [5], anti-convulsant [6], antimalarial [7], antitubercular [8], anti-HIV, anti-inflammatory [9], and antidepressant activities, among others [10]. Their improved lipophilic nature, which increases their bioavailability in lipid membranes and causes growth redundancy in the organism, may be the cause of their increased reported bioactivity [11]. Amino acids [12], 1,2,4-triazole [13], sulfonamides [14], coumarins [15] or resacetophenone, aminothiazolylbromo coumarins, crown ethers [16], and O-Phthaldehyde [17] are other crucial areas of application of this framework that create favorable conditions for utilizing Schiff bases with antimicrobial potential Tetrahydroimidazoles, commonly referred to as imidazolidines (saturated imidazoles), are biologically active heterocyclic compounds that contain nitrogen and have been shown to exhibit a wide range of noteworthy bioactivities [18].

Since they were discovered more than a century ago, imidazolidine-2,4-diones, often known as hydantoins, have gained widespread recognition. Imidazolidine derivatives, also known as hydantoins, are synthetic compounds with a variety of therapeutic uses. Imidazolidines and their derivatives have demonstrated anticonvulsive and antiarrhythmic pharmacological activities [19]. Hydantoins have found therapeutic applications in drugs like the well-known phenytoin [20]. The derivatives of imidazolidine have a significant role in medicinal chemistry due to their wide application as drugs and drug-intermediates [21]. Numerous imidazolidine derivatives have psychopharmacological qualities, such as phenytoin, which is well-known for its effectiveness as an anticonvulsant but is also useful in treating neuropathic pain [22]. Imidazolidine derivatives are present in numerous areas of medicinal chemistry, including antagonists of serotonin and fibrinogen receptors, inhibitors of the NMDA receptor's glycine binding site, antagonists of leukocyte cell adhesion, and allosteric inhibitors of protein–protein interactions [23]. Imidazolidine has two structural isomers: (1,2) and (1,3), Figure 1.

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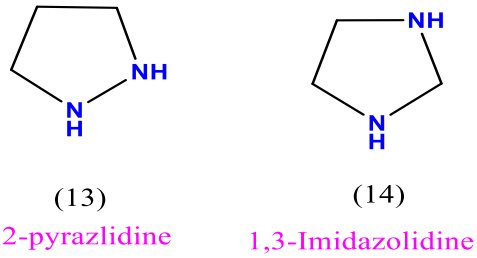

(13) 1,2-pyrazlidine (14) 1,3-Imidazolidine

Figure 1. Imidazolidine isomers structural

This title was chosen depending on type of hetrocyclic synthized compounds and activity tested to this compounds. In this research we used new substituted groups do not used in previous studies that give high activity in synthized compounds. The aim of this study is to prepare new thiadiazole derivaties and to investigate their biological activity as antioxidants, antibacterial agents, and antifungals.

2. Materials and Procedures

1.2 Purchasing and getting ready

Sigma-Aldrich, Fluka, GCC, BDH, S.D. Fine, Scharlau, and Merck purchased synthetic starting ingredients, reagents, and solvents. A single spot-on silica TLC plate with an aluminum background (0.2 mm, 60 F254) was utilized to record the data for each pure component.

2.2 Methods of preparation

2.2.1 Synthesis Amino-1,3,4-thiadiazole-5-thiol [A] [24,25]

10 mL of carbon disulfide was added after 5.3 g, 50 mmol of anhydrous sodium carbonate, and 9.1 g, 100 mmol of thiosemicarbazide were agitated in 50 mL of pure ethyl alcohol for ten minutes. For a full day, the mixture was refluxed at roughly 70 degrees Celsius. After the reaction, a vacuum was used to remove the solvent. The solid was then dissolved in 100 milliliters of distilled water, filtered, and carefully acidified with strong hydrochloric acid to create a yellow solid that was filtered and dried. After that, distilled water was used to recrystallize the white crystalline product (10.64 g, 80%), mp 230–232 ^{o}C, Lit. 231 ^{o}C.

2.2.2.Synthesis of 2-Hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)benzaldehyde (B) [26]

Compound (A) (3.99 g, 30 mmol) was dissolved in a solution of 25 mL of distilled water and 12 mL of HCl. Next, while stirring at 0°C, 2.07 g (30 mmol) of sodium nitrite was added gradually.

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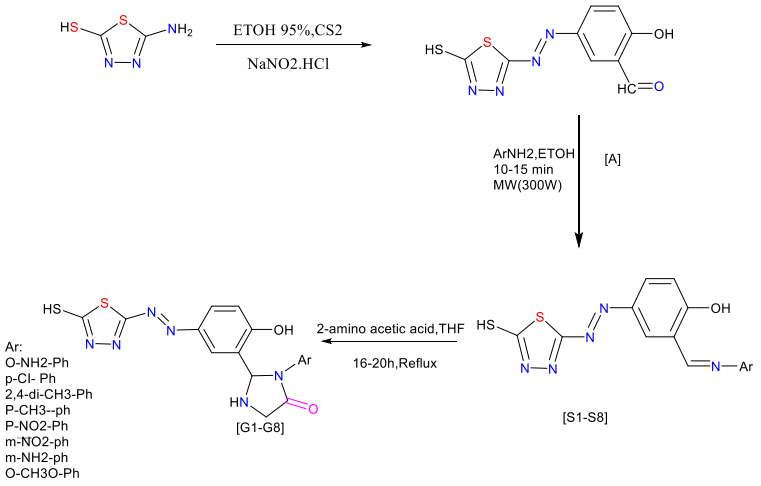
Next, 3.66 g (30 mmol) of salicylaldehyde was dissolved in 25 mL of 10%w/v NaOH at 0°C to create the phenoxide salt. The sodium phenoxide solution was carefully mixed with the diazonium chloride solution. The solution was allowed overnight to complete the precipitation process once addition was complete. Ethyl alcohol recrystallized the orange solid, yielding (2), yield (4.63g,58%), m.p. 189-191ºC.

2.2.3. Synthesis of azoimines derivatives S_1-S_8 [27]

In an home microwave oven set to 300W for 15 minutes on a crucible, compound (B) (0.266 g, 1 mmol) and substituted phenyl amines (1 mmol) were combined with 1 mL of pure ethyl alcohol. Reactions have been completed using TLC (n-hexane: EtOAc, 1:2). Crude products were recrystallized using ethanol. Table (2-2) shows certain physical properties and other features for goods (S_1-S_8).

2.2.4. Synthesis of imidazolin-4-ones derivatives G_1-G_8 [28]

After stirring a mixture of Schiff bases (S1-S8) (0.0021 mol) in 9 mL of THF solvent, 2-aminoacetic acid (0.25 g, 0.0021 mol) in 5 mL of THF was refluxed for 16–20 hours. After cooling to room temperature, the liquid was filtered, cleaned, and recrystallized from acetone. Table 1 physical characteristics of compounds (G_1–G_8).



Scheme 1. Synthesis of derivatives of imidazolin-4-ones G_1–G_8 .

Scheme 2 illustrates the suggested chemical mechanism for ring closure that results in imidazolin-4-one in a THF solution.

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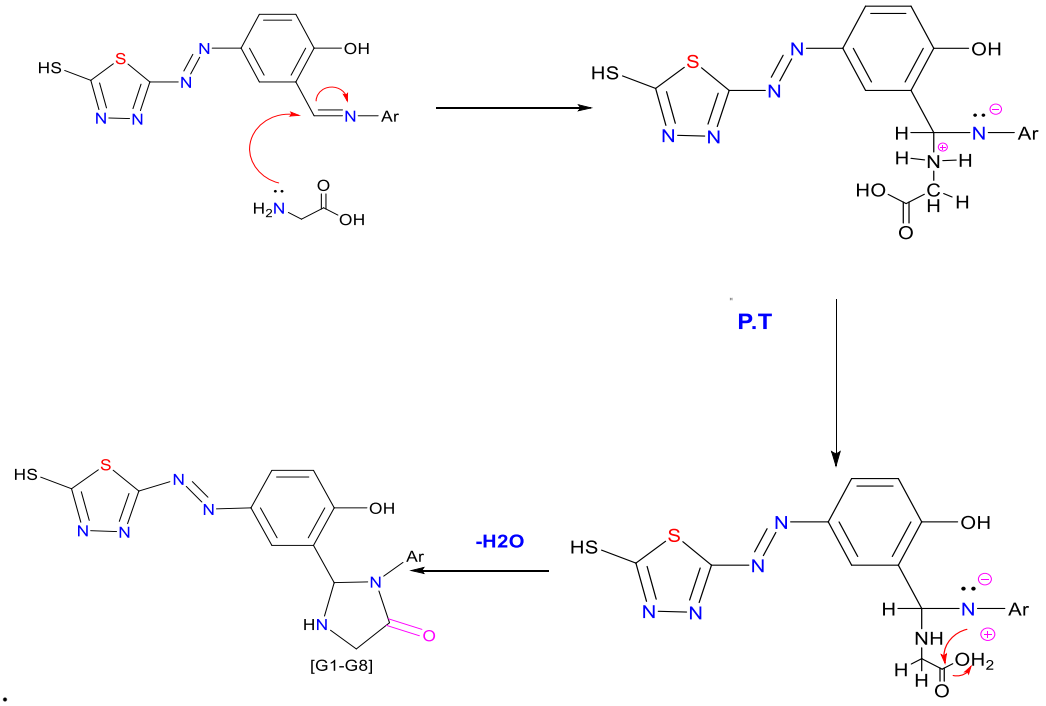

Scheme 2.The creation of imidazolin-4-ones G_1-G_8 in THF.

Table 1.Physical characteristics of every synthetic chemical substance.

Compound No.	Color	Rf *n*-hexane/EtOAc(1:2)	m.p. (^oC)	Yield (%)
S_1	Dark brown	0.73	173-175	88
S_2	Orange	0.82	132-134	80
S_3	Dark red	0.62	154-156	76
S_4	Dark red	0.69	169-171	73
S_5	yellow	0.72	141-143	85
S_6	red	0.67	152-154	76
S_7	yellow	0.79	141-143	85
S_8	yellow	0.84	121-123	72
G_1	Dark brown	0.58	199-201	95
G_2	brown	0.69	212-214	89
G_3	Dark brown	0.51	163-165	81
G_4	light brown	0.55	174-176	90

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G_5	Dark brown	0.53	150-152	88
G_6	light brown	0.56	168-170	90
G_7	Dark brown	0.59	155-157	86
G_8	light brown	0.61	178-180	91

2.3. Antibacterial activity

The antibacterial activity of the target 5-substituted Imidazolin-4-one compounds G1-G8 was assessed using *Staphylococcus aureus* (Gram-positive) and Escherichia coli (Gram-negative) bacteria using the agar diffusion technique [29]. Exact 1.25, 2.5, 5, 10, 15, and 20 mg of each investigated chemical were resolved in 1 milliliter of DMSO. Gentamycin, the reference antibiotic, was used as a control medication to compare the inhibitory zone results. Pure cultures of Staphylococcus aureus and Escherichia coli, were subcultured on appropriate media and incubated at 37 °C for 18–24 hours. Colonies were suspended in sterile saline and adjusted to 0.5 McFarland standard. Each investigated compound's inhibitory zone is displayed in Table 2 .

Table 2. Imidazolin-4-one derivatives G_1–G_8's antibacterial activity

Compound No.	***Concentration***	**Bacteria Type**	
		Staphylococcus Aureus (G+)	***Escherichia Coli (G-)***
		Inhibitory zone (diameter) (mm)	
G_1	1.25	NO	NO
G_1	2.5	10.1	8.8
G_1	5	12.5	11.7
G_1	10	17	14.9
G_1	15	18.9	20.3
G_1	20	19.9	22.2
G_2	1.25	NO	NO
G_2	2.5	7.8	10
G_2	5	9.1	10.6
G_2	10	16.5	15.9
G_2	15	19.2	19.5
G_2	20	28.2	20.8

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G_3	1.25	NO	NO
G_3	2.5	8.2	8.9
G_3	5	8.9	9.4
G_3	10	15.2	15.8
G_3	15	19.7	19
G_3	20	23.1	24.5
G_4	1.25	NO	NO
G_4	2.5	10	8.6
G_4	5	10.6	9.7
G_4	10	16.1	15
G_4	15	18.8	19.3
G_4	20	29.8	28.1
G_5	1.25	NO	NO
G_5	2.5	9.5	8.8
G_5	5	10.2	9.3
G_5	10	15.9	15
G_5	15	19.5	19.6
G_5	20	26.5	21.2
G_6	1.25	NO	NO
G_6	2.5	9.1	8.4
G_6	5	9.8	9.8
G_6	10	15.2	15
G_6	15	18.9	19.4
G_6	20	22.7	20.5
G_7	1.25	NO	NO
G_7	2.5	8.7	9.2
G_7	5	9.5	10.4
G_7	10	15.4	15.7
G_7	15	19.7	19.2
G_7	20	28.3	26.2
G_8	1.25	NO	NO

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G_8	2.5	7.6	9.5
G_8	5	8.4	9.9
G_8	10	16.1	17.4
G_8	15	19.7	20.5
G_8	20	25.3	28.6
DMSO	-	-	-
Gentamycin	-	18	15

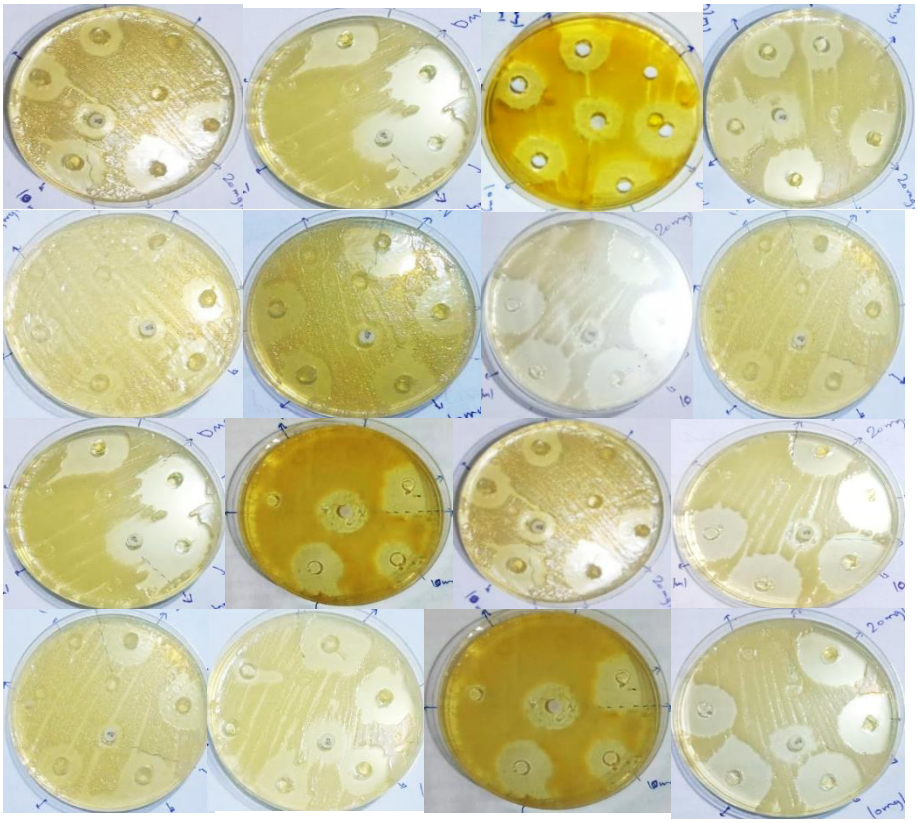

Figure 2. Inhibition zone of compounds G_1-G_8 on gram-negative and gram-positive bacteria

2.3. Antfungial activity

Candida fungus were used to assess the antifungal activity of the target 5-substituted Imidazolin-4-ones compounds G1-G8 using the agar diffusion technique [29]. Exact 1.25, 2.5, 5, 10, 15, and

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20 mg of each investigated chemical were resolved in 1 mL of DMSO. The reference antibiotic, nystatin, was used as a control medication to compare the inhibitory zone results. Pure cultures of Candida albicans were subcultured on appropriate media and incubated at 37 °C for 48 hours. Colonies were suspended in sterile saline and adjusted to 0.5 McFarland standard. Each investigated compound's inhibitory zone is displayed in Table 3.

Table 3. Imidazolin-4-one derivatives G_1–G_8's antifungal activity.

Compound No.	***Concentration***	**Candida**
		Inhibitory zone (diameter) (mm)
G_1	1.25	NO
G_1	2.5	6.9
G_1	5	8.6
G_1	10	16.8
G_1	15	19.1
G_1	20	22.0
G_2	1.25	NO
G_2	2.5	6.4
G_2	5	9.6
G_2	10	16.8
G_2	15	18.9
G_2	20	25.4
G_3	1.25	NO
G_3	2.5	6.6
G_3	5	7.9
G_3	10	16.1
G_3	15	18.7
G_3	20	22.2
G_4	1.25	NO
G_4	2.5	6.8
G_4	5	7.7
G_4	10	16.5

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G_4	15	18.2
G_4	20	29.9
G_5	1.25	NO
G_5	2.5	6.6
G_5	5	8.5
G_5	10	16.3
G_5	15	18.1
G_5	20	24.8
G_6	1.25	NO
G_6	2.5	6.1
G_6	5	8.3
G_6	10	16.7
G_6	15	18.5
G_6	20	20.2
G_7	1.25	NO
G_7	2.5	6.4
G_7	5	8.1
G_7	10	16.4
G_7	15	18.1
G_7	20	28.2
G_8	1.25	NO
G_8	2.5	6.1
G_8	5	7.5
G_8	10	17.5
G_8	15	18.5
G_8	20	27.9
DMSO	-	-
Nystatin	-	21

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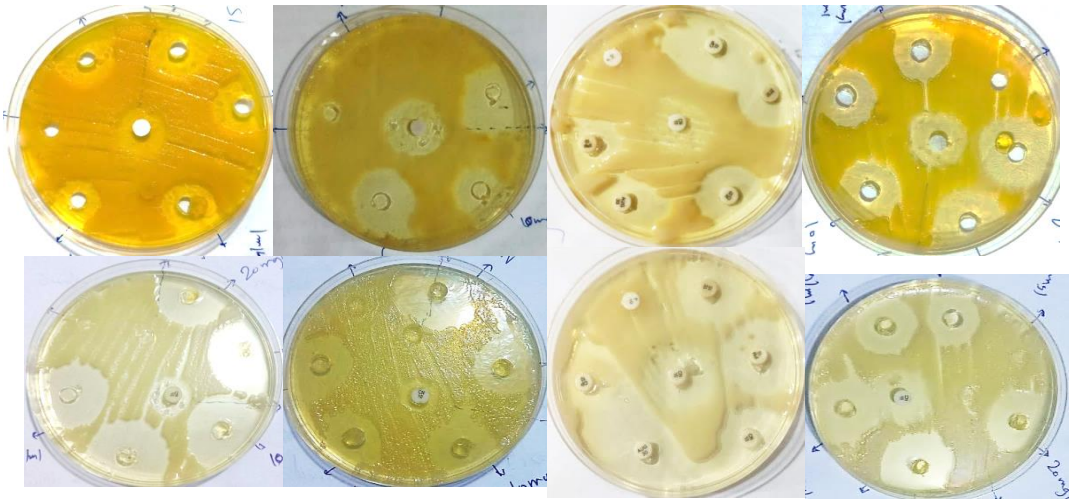

Figure 3.Inhibition zone of compounds G_1-G_8 on candida

2.4.Determination of antioxidant activity

Using ascorbic acid as the standard solution, the DPPH assay was used to examine how well the produced compounds G1–G8 scavenged free radicals in vitro. Four milligrams of DPPH were dissolved in one hundred milliliters of ethanol to create a standard DPPH solution. Then, 200 µL of each of the tested substances at varying concentrations were combined with 1000 µL of the DPPH solution. The absorbance was measured at a wavelength of 517 nm using ethanol as a blank after the mixtures were incubated for 30 minutes at room temperature in the dark. The reference standard was ascorbic acid [30]. The following formula was used to get the percentage of DPPH free radical (% Inhibition):

$$\%\mathbf{Inhibition} = \left[\frac{A^\circ - A1}{A^\circ}\right] \times 100 \qquad \ldots (1)$$

Where: A° is the DPPH solution's absorbance in the absence of the sample

A1 is the absorbance of the tested substance

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3.Findings and conversation

3.1 Chemistry

Imidazolin-4-one derivatives G_1–G_8 were synthesized utilizing an effective approach that utilized reflux conditions (Scheme 1). The product is produced rapidly and with a high yield by this technically straightforward reaction. The hydrogens at positions 1 and 3 in the 1H NMR spectra are the signals that demonstrate the creation of the imidazolin-4-one ring (Figure 4)

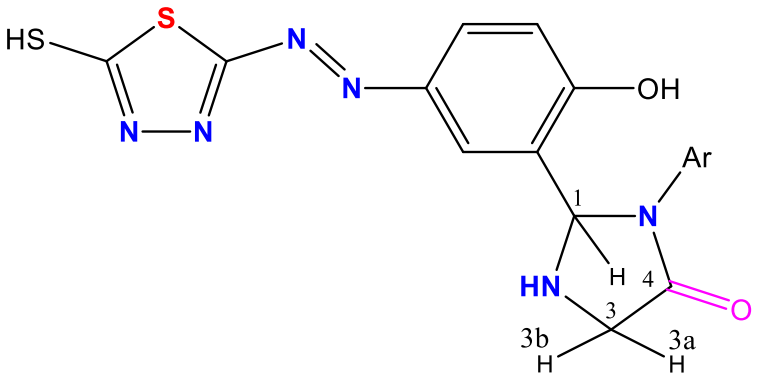

Figure 4. The synthetic imidazolin-4-one ring's general skeleton.

The hydrogen 3, a member of the asymmetric carbon 3, is another distinctive signal that manifests as singlet signals between 3.5 and 4 ppm. Carbons 1, 3, and 4 are the characteristic peaks in the 13C NMR spectra of imidazolin-4-one. At roughly 165–175 ppm, the carbonyl carbon 4 is the most deshielded signal in the spectrum. Methylene carbon 1 displays a sign in the range of 65–75 ppm, while carbon 3 shows at 46–52 ppm. (S_1-S_8) do not identification in ^{1}HNMR and ^{13}CNMR because the are previous preparation in previous studies .Detailed illustrations of other signals are provided:

2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)-3-(p-tolyl)imidazolidin-4-one (G_1, $C_{18}H_{16}N_6O_2S_2$).^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm, *J*H-H = Hz): 13.5-14.5(s,1H , S-H) ,10.5- 11.5 (s,,1H, Ar-OH),8.5-9.5 (s,1H,-NH Imidazolidinone),8.0-8.2(d ,1H , Ar-H) , 7.7-7.9(dd,1H,Ar-H),7.3-7.5(d,2H,P-tolyl Ar-H),7.1-7.2(m,3H, Ar-H (Tolyl and Phenol) Overlapping)),5.8-6.2(s,1H,-CH-Imidazolidinone Methine), 3.5- 4.0(s,2H, ,-CH Imidazolidinone Methylene),2.2-2.3(s,3H,CH_3methyl group).

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^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 171.43 (C=O Imidazolidinone), 163.80(C-N=Nthiadiazole), 162.66(C-SH), 156.94(Ar-C-OH), 142.39(C-N=N),133.33(C-CH_3),115-130(Ar-C), 65 – 75 (N−CH−N imidazolidinone rin), 46.16(-CH imidazolidinone ring**)** and 20.09(-CH_3 methyl group) **.**

3-(2,4-dimethylphenyl)-2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)imidazolidin-4-one(G_2,$C_{19}H_{18}N_6O_2S_2$) ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm, *J*H-H = Hz): 13.0-14.50(s,1H , S-H) ,10.5- 11.5 (s,,1H, Ar-OH),9.0-10.5 (s,1H,-NH Imidazolidinone),6.70-8.20(m ,6H , Ar-H),5.80-6.50(s,1H, -CH-Imidazolidinone Methine), 3.60-4.0(s,5H, Ar-H,-CH Imidazolidinone Methylene),2.20-2.40(s,3H,CH3methyl group).

^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 173.25(C-SH), 168.18 (C=O Imidazolidinone), 163.09(C=Nthiadiazole), 155.44(Ar-C-OH), 151.08(C-O-CH3) , 119.48(Ar-C),110-130(Ar-C), 65.85 (N−CH−N imidazolidinone ring), 49.10 (-CH imidazolidinone ring**)** and 20.59(-CH_3 Methyl substituent**)**.

2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)-3-(3-hydroxyphenyl)imidazolidin-4-one (G_3, $C_{17}H_{14}N_6O_3S_2$).^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm, *J*H-H = Hz): 13.5-14.2 (s,1H , S-H) ,10.2- 11.0 (s,,1H, Ar-OH), 9.2-9.8(s,1H,Ar-H),8.5-9.2(s,1H,-NH Imidazolidinone), 8.0-8.3(d ,*J=2*,1H,Ar-H) ,7.8-8.0 (d , 1 H , Ar-H) ,7.0-7.2 (d , *J=2*,1H , Ar-H), 6.5-7.4(m ,5H , Ar - H) , 5.8-6.5 (s,1H,-CH-Imidazolidinone Methine),3.6- 4.0(s,2H, ,-CH Imidazolidinone Methylene).

^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 167.80(C=S thiadiazole), 165-175 (C=O Imidazolidinone), 162.11(C-N=N thiadiazole), 158.36(Ar-C-OH),139.83(C-N),126.75(Ar-C), 114.76(Ar-C),70.05 (N−CH−N imidazolidinone ring) and 47.56 (-CH imidazolidinone ring **) .**

2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)-3-(2-hydroxyphenyl)imidazolidin-4-one (G_4, $C_{17}H_{14}N_6O_3S_2$).^{1}H NMR (500 MHz, DMSO-d6) δ (ppm, JH-H = Hz): 13.5-14.2(s,1H,S-H),10.5-11.5 (s,,1H, Ar-OH)9.0-10.5(s,1H,Ar-OH),7.8-8.2 (d ,2H , Ar-H), ,6.7-7.6 (m ,5H ,Ar-OH)5.8 - 6.4(d,1H ,-CH Imidazolidinone Methine),4.5 - 5.5(s,1H, -NH- Imidazolidinone Amine),3.5-4.2(m,2H,-CH Imidazolidinone Methylene).

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^{13}C NMR (125 MHz, DMSO-d6) δ (ppm): 173.35 (C=O Imidazolidinone), 162.34(C-SH),160.89(Ar-C-OH), 152.58(C-N=Nthiadiazole), 134.73(C-N imidazolidinone ring),115-130(Ar-H), 66.81 (N−CH−N imidazolidinone ring), and 46.30 (-CH imidazolidinone ring).

2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)-3-(3-nitrophenyl)imidazolidin-4-one (G_5, $C_{17}H_{13}N_7O_4S_2$).^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm, *J*H-H = Hz:13.5-14.5(s,1H , S-H) ,10.5- 11.5 (s,,1H, Ar-OH),8.5-10.5(s,1H,-NH Imidazolidinone), 8.5-8.7(s ,1H,Ar-H) ,8.0-8.2 (m ,, 1 H , Ar-H),7.6-7.9 (m ,2H , Ar-H), 7.8-8.1(s ,1H , Ar - H) , 6.9 - 7.5 (dd , *J=8,2* , 2H , Ar-H),6.2-6.6 (s,1H,-CH-Imidazolidinone Methine),3.6- 4.0(s,2H, ,-CH Imidazolidinone Methylene).

^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 171.07 (C=O Imidazolidinone), 163.33(C-SH), 159.14(C-N=N thiadiazole), 157.98(Ar-C-OH), 150.00(C-NO2),143.82(C-N=N),140-145(C-N), 110-135(Ar-C),70.79 (S−CH−N imidazolidinone ring) and 52.27 (-CH imidazolidinone ring **) .**

2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)-3-(2-methoxyphenyl)imidazolidin-4-one (G_6, $C_{18}H_{16}N_6O_3S_2$).^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm, *J*H-H = Hz): 13.5-14.2 (s,1H , S-H) ,10.0- 10.8 (s,,1H, Ar-OH), 7.8 - 8.2 (d , 2H , Ar-H) , 6.8-7.6 (m,6H,Ar-H), 6.0-6.3 (s,1H,-CH-Imidazolidinone Methine), 4.2-5.0(s,1H,-NH Imidazolidinone), 3.75(s ,3H,OCH_3) , 3.5- 3.8(s,2H, ,-CH Imidazolidinone Methylene).

^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 169.68 (C=O Imidazolidinone), 162.52(C=N thiadiazole),157.99(Ar-C-OH),153.62(C-O-CH3),127.10(C-N),112-135(Ar-C),66.41 (N−CH−N imidazolidinone ring), 55.51(O-CH3)and 49.94 (-CH imidazolidinone ring **) .**

2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)-3-(4-nitrophenyl)imidazolidin-4-one (G_7, $C_{17}H_{13}N_7O_4S_2$).^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm, *J*H-H = Hz): 13.5-14.5(s,1H , S-H) ,10.5- 11.5 (s,,1H, Ar-OH),8.2-8.3(d , *J=9* ,2H,Ar-H) ,7.8-8.0 (d , *J=9*, 2 H,Ar-H),7.6-7.9 (d, 1H, Ar-H), 7.1-7.4(m ,1H,Ar-H),6.8-7.1(d,1H,Ar-H),6.0-6.5 (s,1H,-CH-Imidazolidinone Methine), 4.5-5.5(s,1H,-NH Imidazolidinone),3.5- 4.0(s, 2H, ,-CH Imidazolidinone Methylene).

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^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 171.69(C=S), 169.24 (C=O Imidazolidinone), 162.36(C=N thiadiazole), 156.90(Ar-C-OH), 148.80(C-N) ,141.40(C-NO_2),126-135(Ar-C), 115-135(Ar-C), 66.09(N−CH−N imidazolidinone ring) and 46.85 (-CH imidazolidinone ring **) .**

3-(4-chlorophenyl)-2-(2-hydroxy-5-((5-mercapto-1,3,4-thiadiazol-2-yl)diazenyl)phenyl)imidazolidin-4-one(G_8, $C_{17}H_{13}ClN_6O_2S_2$).^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm, *J*H-H = Hz): 13.5-14.2(s,1H,S-H),10.5- 11.5 (s,,1H, Ar-OH)9.0-10.5(s,1H,Ar-OH),7.8-8.2 (d ,2H , Ar-H), ,6.7-7.6 (m ,5H ,Ar-OH)5.8 - 6.4(d,1H ,-CH Imidazolidinone Methine) ,4.5 - 5.5(s,1H , -NH- Imidazolidinone Amine),3.5-4.2(m,2H,-CH Imidazolidinone Methylene).

^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 169.99 (C=O Imidazolidinone), 163.12(C-N=Nthiadiazole), 159.80(C-SH), 155.10(Ar-C-OH), 146.72(C-N=N azo),128.28(C-Cl), 66.75 (N−CH−N imidazolidinone ring), and 51.53 (-CH imidazolidinone ring**).**

Tables 4 and 5 display the FT-IR spectrum and analytical data for the synthesized compounds A,B, S_1-S_8, and G_1-G_8.

Table 4. Compounds A, B, and S1-S8's FT-IR spectrum data (cm^{-1})

Compound no.	A	B	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8
ν(O-H)	-	3421.83	3414.12	3450	3400-2500	3194	3446-3358	3441.12	3458.48	3414.12
ν(C-H) aromatic	-	3060	3100	3050	3090	3194	3010	3161.43	3184.58	3167.22
ν(C=O)	-	1637.62	-	-	-	-	-	-	-	-
ν(C=N) imine	-	-	1618.33	1535	1616.47	1599.04	1627.97	1535.39	1614.47	1612.54
ν(C=N) thiadiazole	1597	1618.33	1618.33	1535	1616.47	1599.04	1627.97	1535.39	1535.39	1612.54
ν(C=C) aromatic	-	1550.82	1539.25	1504.53	1535	1492,1448	1595.18	1504.53-1398.44	1535.39 - 1500.47	1539.25- 1491.
ν(N=N)		1489.10	1402.30	1504.53	1535	1566.25	1595.18	1504.53	1500.47	1454.38

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δ o.o.p (C-H) aromatic	-	831.35	812.02	812.06	835.21	837.13	842.92	812.06	750.33	856.42
Other bands (v)	3399,3281 (NH2)	1217(C-O)	2926 (C-H)alphatic	2889 (C-H)alphatic	1282 (C-O)	1290 (C-O)	1487,1329 (NO2)	1215.19 (C-O)	1460.16 - 1319.35 (NO2)	725.26 (C-Cl)

Table 5. Imidazolin-4-ones G1-G8 FT-IR spectrum data (◦, cm^{-1})

Compound No.	**G_1**	**G_2**	**G_3**	**G_4**	**G_5**	**G_6**	**G_7**	**G_8**
ν(O-H)	3400	3400-3100	3400-2400	3500-2500	3400-3100	3400	3414	3400-3100
ν(C-H) aliphatic	2953	2953	2964	2874	2989-2872	2953	2885	2968-2843
νC-H) aromatic	3160	3130	2964	2993	3074	3100	3074	3150
ν(C=O)	1690	1689	1691	1689	1691	1691	1700	1689
ν(C=N) thiadiazole	1599	1649	1645	1608	1643	1604	1597	1604
ν(C=C) benzene	1508	1512-1421	1475	1608	1600-1421	1604	1458-1425	1604
ν(N=N)	1599	1421	1475	1480	1643	1604	1597	1518
ν(S-H) thiol form	2500	2661	2656	2550	2656	2511	2549	2505
Other bands (v)	1247(C-O)	1229(C-O)	1151(C-O)	1041(C-O)	1508-1309(NO2)	750(o.o.p.CH)	1527-1290(NO2)	898(o.o.p CH)

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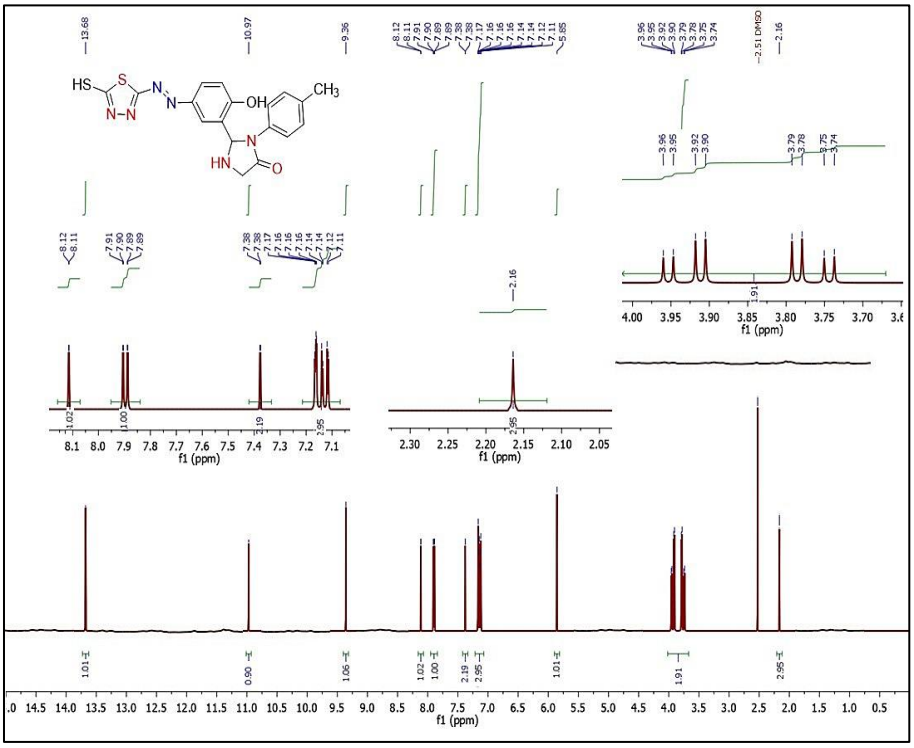

Figure 5. ^{1}H NMR spectrum of compound G_1

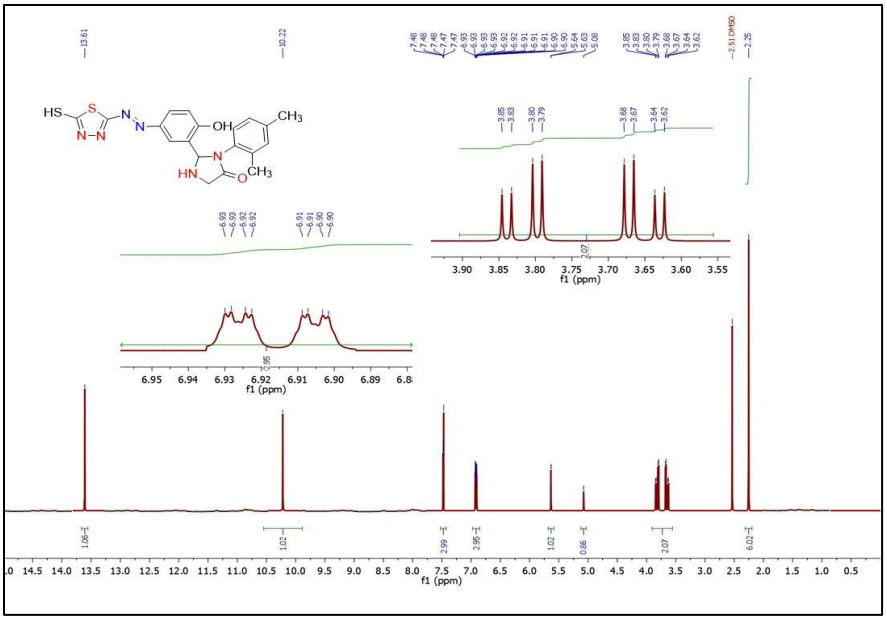

Figure 6. ^{1}H NMR spectrum of compound G_2

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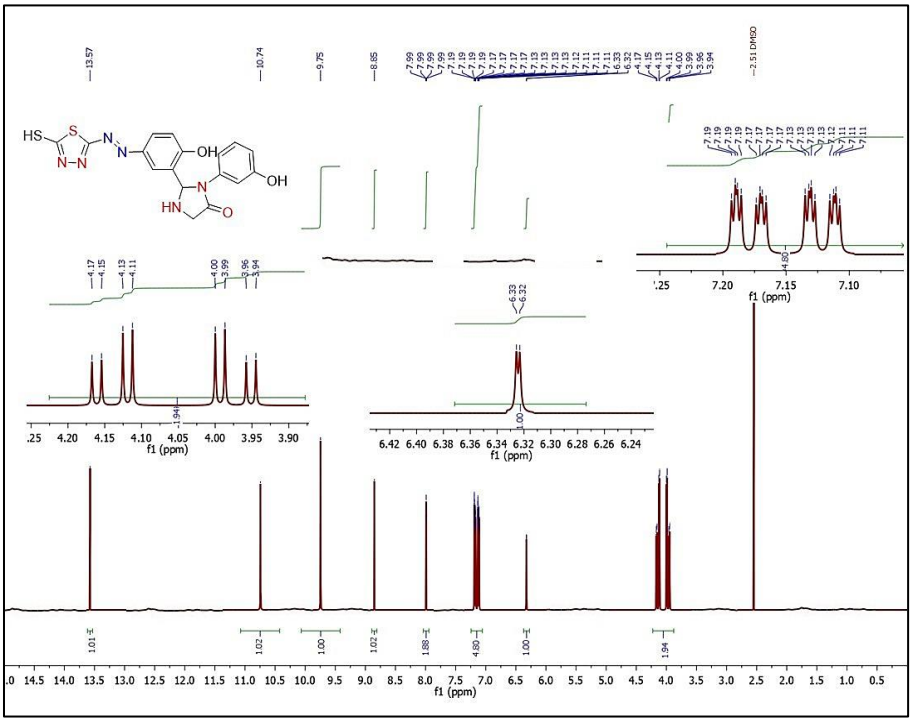

Figure 7. ^{1}H NMR spectrum of compound G_3

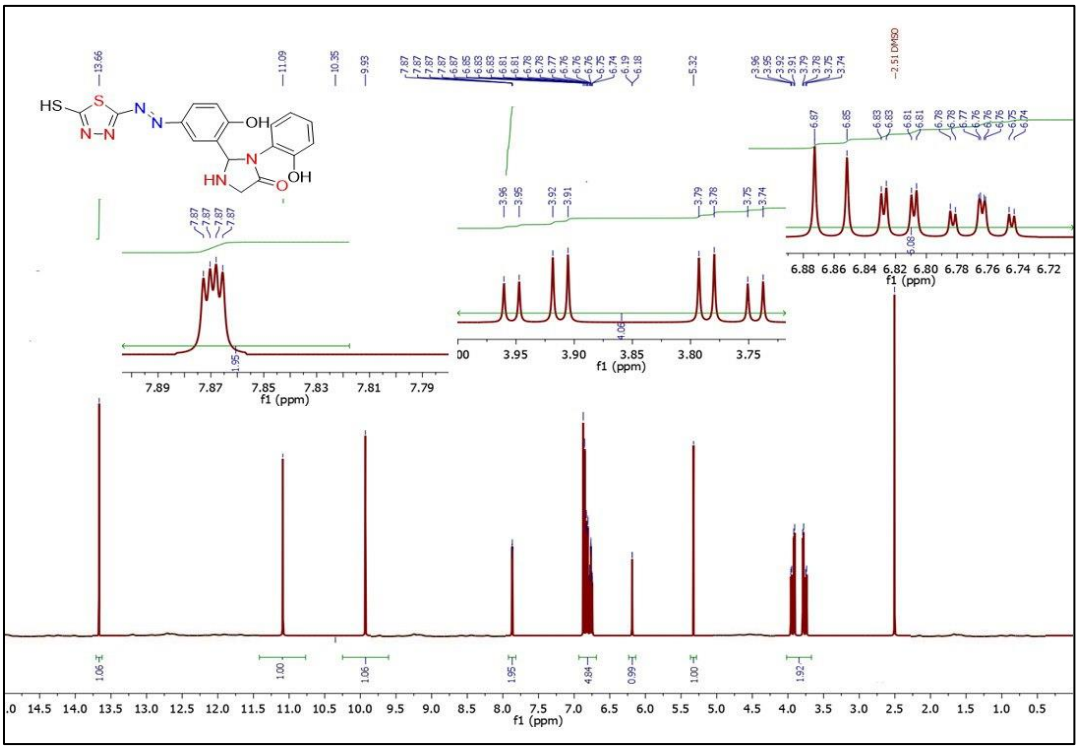

Figure 8. ^{1}H NMR spectrum of compound G_4

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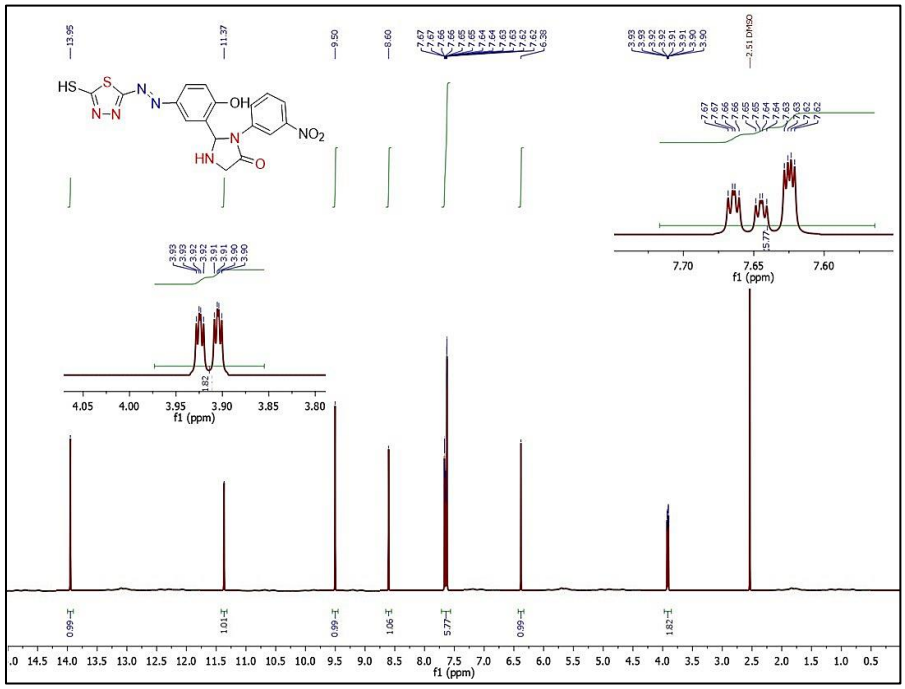

Figure 9. ^{1}H NMR spectrum of compound G_5

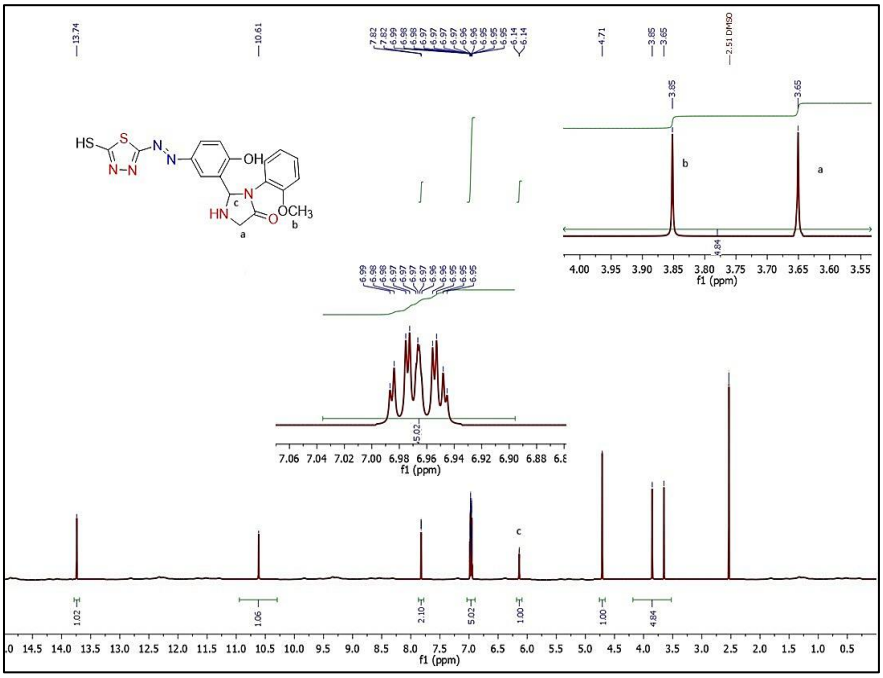

Figure 10. ^{1}H NMR spectrum of compound G_6

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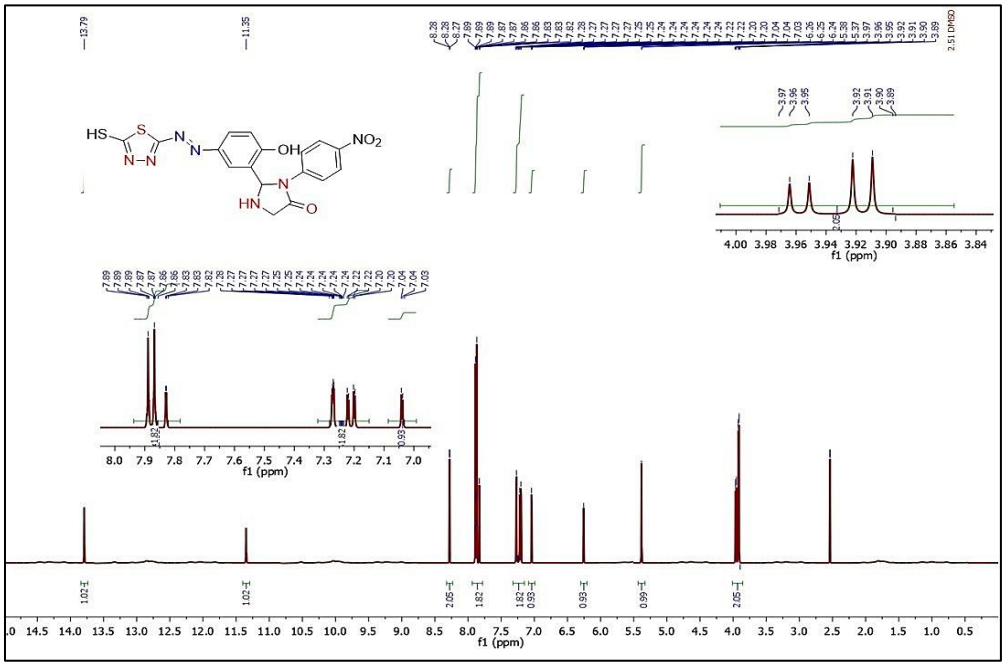

Figure 11.^{1}H NMR spectrum of compound G_7

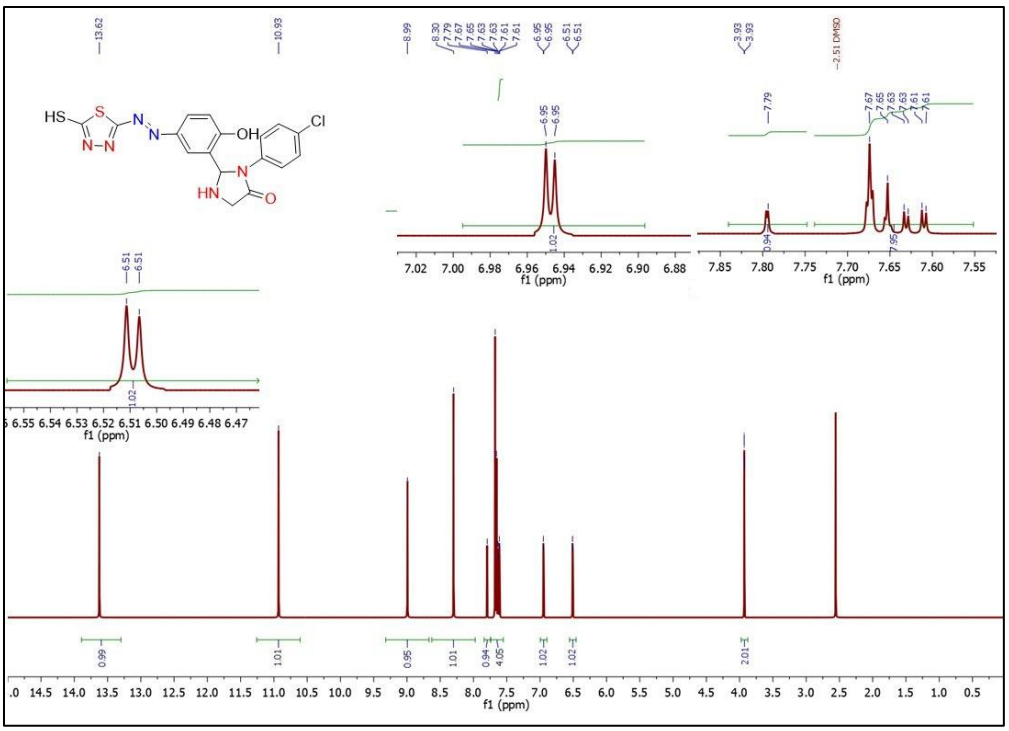

Figure 12. ^{1}H NMR spectrum of compound G_8

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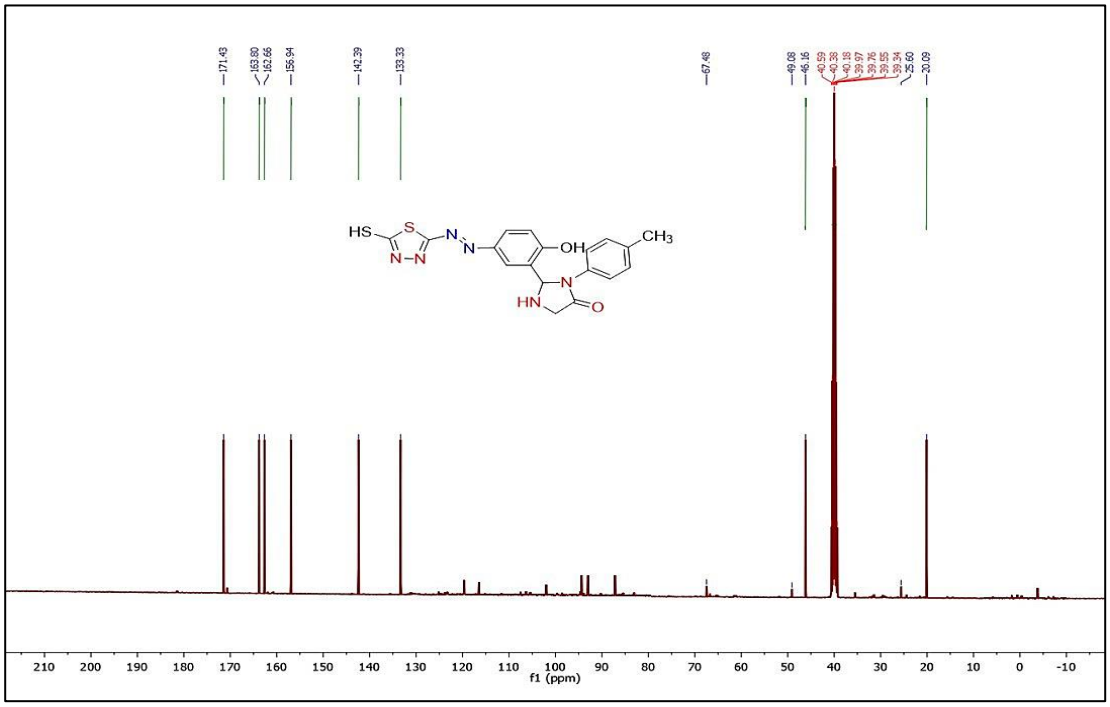

Figure 13. ^{13}C NMR spectrum of compound G_1

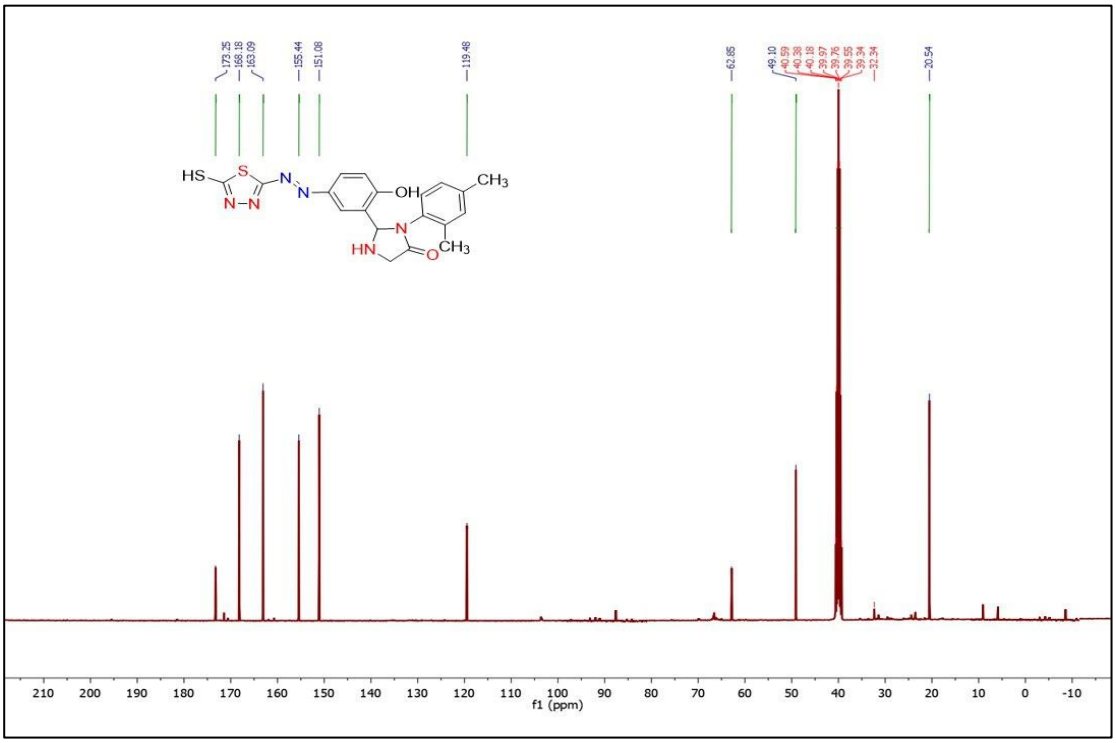

Figure 14. ^{13}C NMR spectrum of compound G_2

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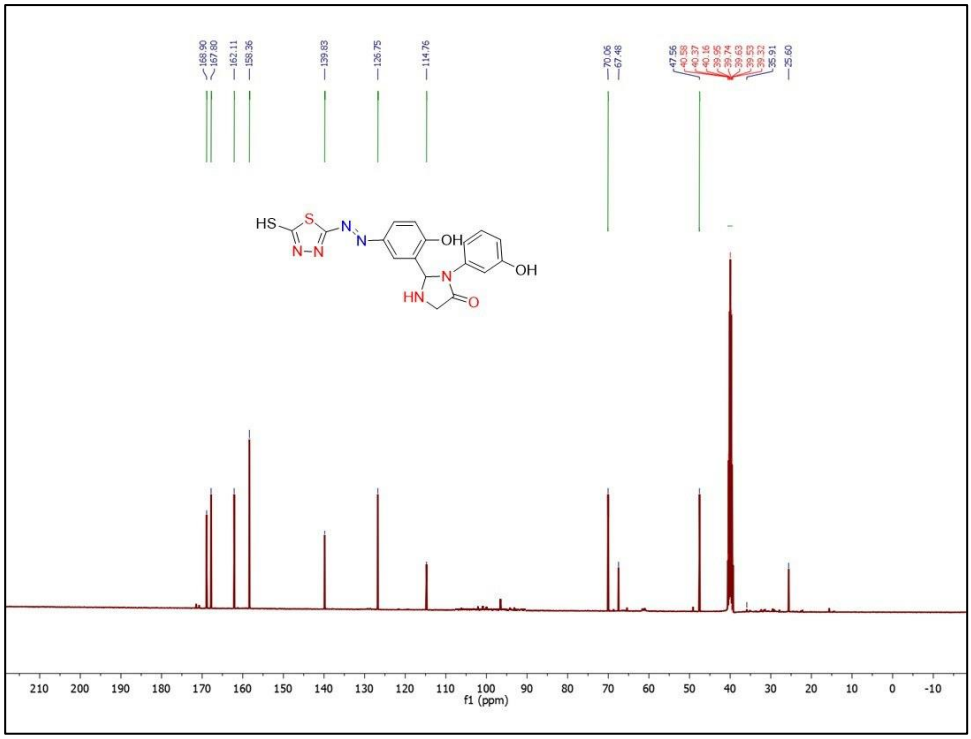

Figure 15. ^{13}C NMR spectrum of compound G_3

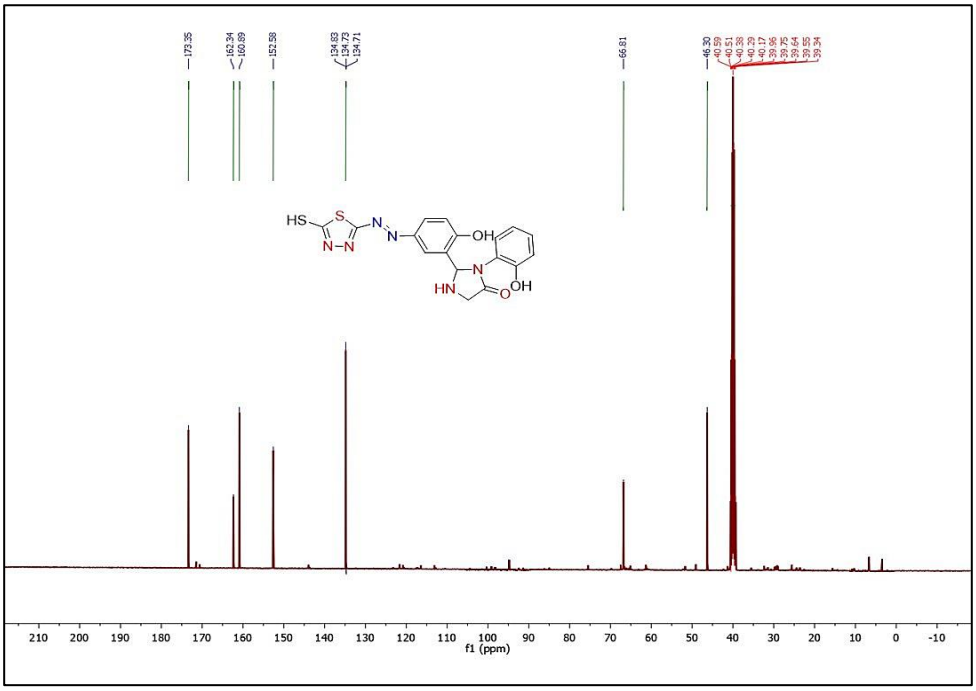

Figure 16. ^{13}C NMR spectrum of compound G_4

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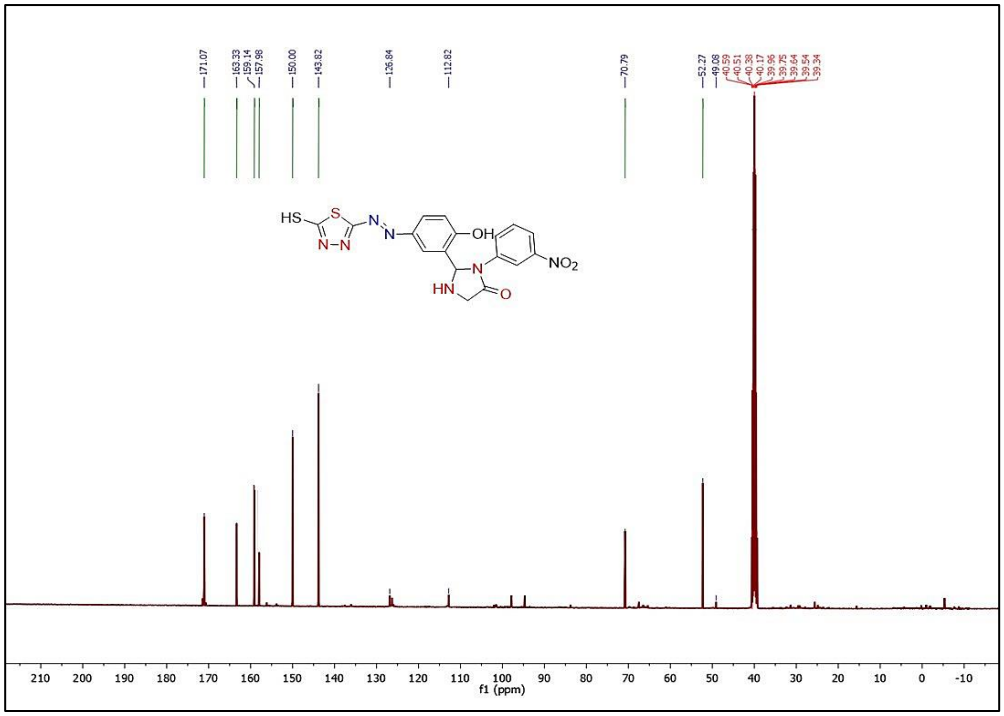

Figure 17: ^{13}C NMR spectrum of compound G_5

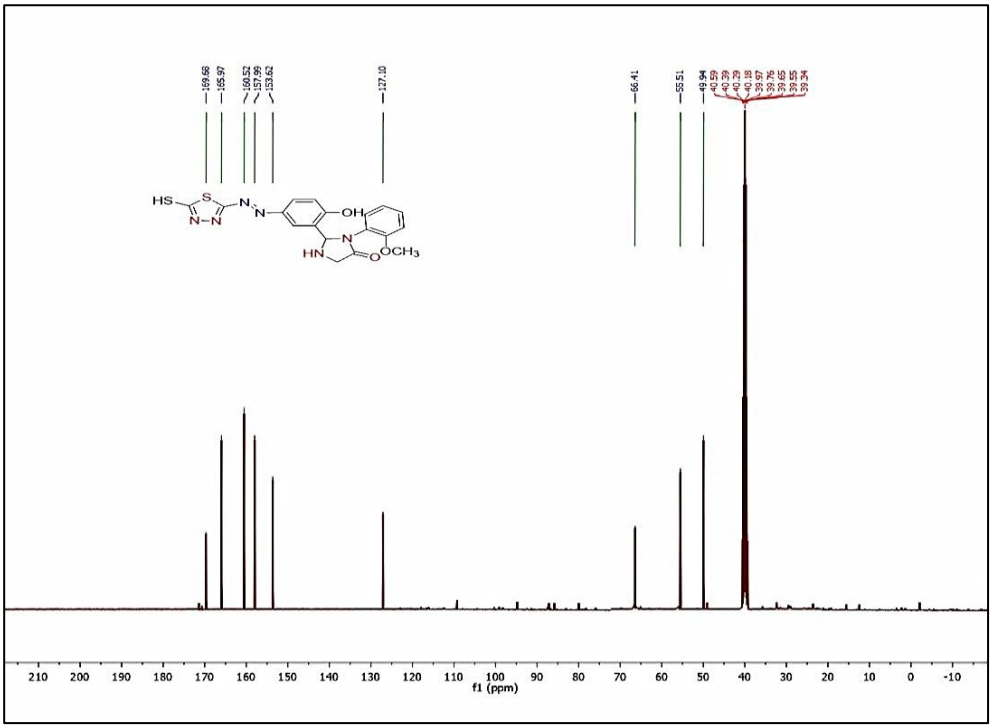

Figure 18. ^{13}C NMR spectrum of compound G_6

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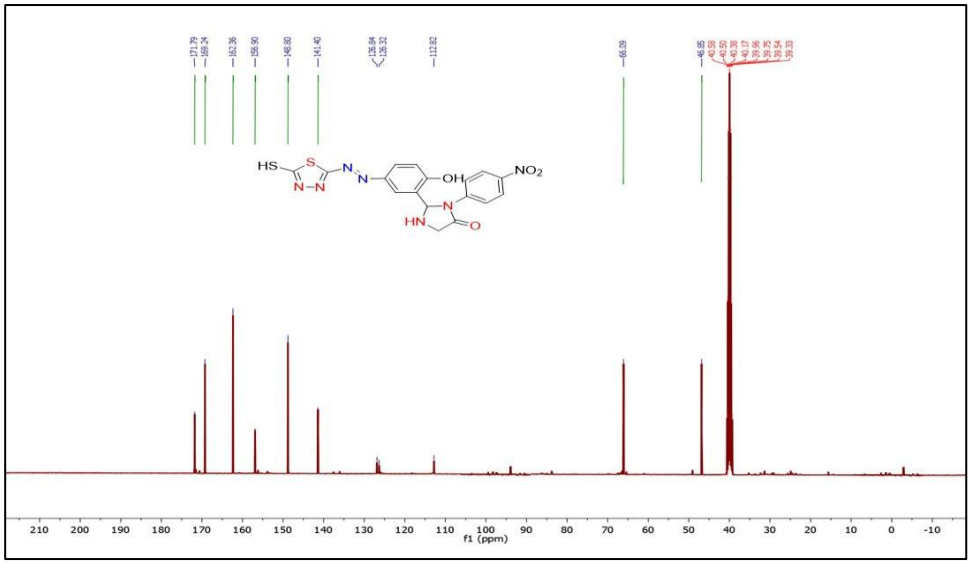

Figure 19. ^{13}C NMR spectrum of compound G_7

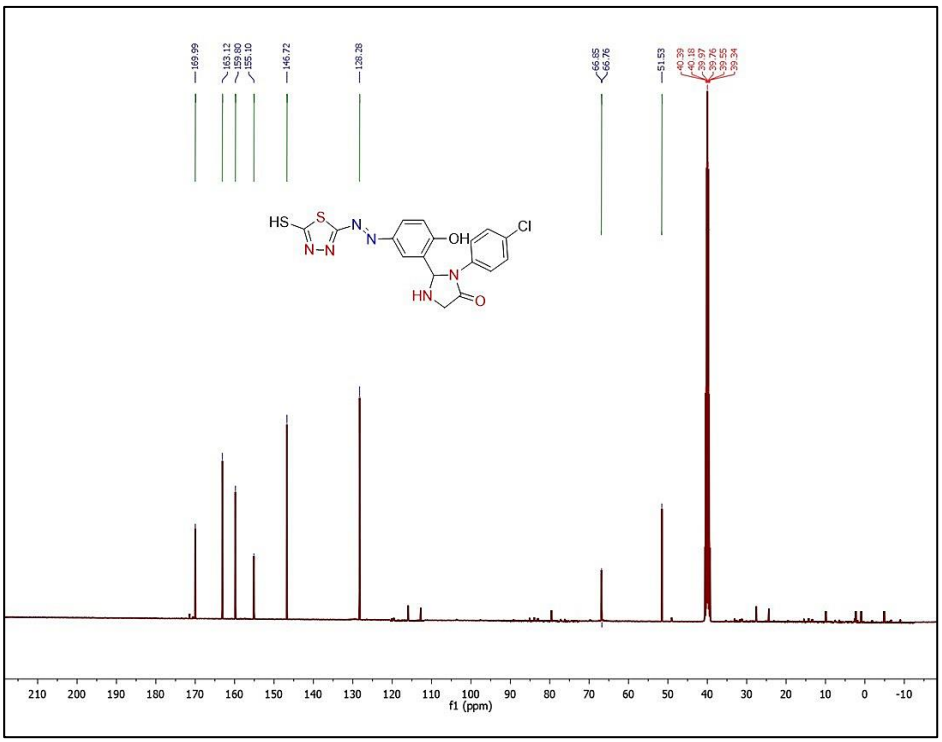

Figure 20.^{13}C NMR spectrum of compound G_8

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3.2.Biological techniques

3.2.1. Activity against bacteria

The antibacterial activity of the generated compounds was assessed against *Escherichia coli*, a gram-negative bacterium, and Staphylococcus aureus, a gram-positive bacterium, using the diffusion method [28]. Imidazolin -4-one derivatives were found to be more effective than Gentamycin as a control medication against Escherichia coli and Staphylococcus aureus in an antibacterial investigation.

3.2.2Activity against fungus

The synthesized compounds' antifungal efficacy against *Candida* fungus was assessed using the diffusion method [28]. Imidazolin-4-one derivatives were found to be more effective than nystatin as a control medication against Candida in an antifungal investigation.

3.2.3. The DPPH test

The generated compounds' antioxidant activity is investigated using the DPPH method. The reducing abilities of the investigated compounds were measured by their capacity to change the purple 1,1-diphenyl-2 picrylhydrazyl radical (DPP•) into its light-yellow reduced form (DPPH). A decrease in violet color was seen at 517 nm, and the absorbance reduction correlates with the substance's antioxidant activity. Utilizing ascorbic acid at concentrations of 50, 100, 150, 200, and 250 mg/mL as the control material, compare the outcomes. The findings show that all drugs performed exceptionally well at the 250 mg/mL concentration. Compounds G_3 (86%), G_4 (88%), and G_6 (85%) have exceptionally potent DPPH radical scavenging properties that are on par with ascorbic acid (85%). The H• of the investigated molecule is transferred to the N• of the DPPH radical reagent via SET and/or HAT kinds of antioxidant processes [31]. One possible location for H atom donation is the hydrogens at the C3 positions of the Imidazolidin-4-one ring, a five-membered heterocyclic ring. This ring's antioxidant activity must result from the straightforward transfer of a H atom to the radicals; the most widely used mechanism is hydrogen atom transfer (HAT). The Imidazolidin-4-one derivatives exhibit antioxidant effects primarily attributed to resonance effects and tautomeric equilibrium. The scavenging activities of synthesized compounds G1-G8 are presented in Table 6 and Graph 1.

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Table 6. The percentages of free radical-scavenging activity for the prepared compounds G_1 through G_8.

Compounds	G_1	G_2	G_3	G_4	G_5	G_6	G_7	G_8
Conc. mg/mL	*Scavenging activity (%)*							
50	60	58	67	70	52	65	71	74
100	65	63	72	74	60	71	74	78
150	71	69	76	79	63	76	80	80
200	79	75	81	80	69	79	82	81
250	81	80	86	88	70	85	83	84
Ascorbic acid 50 µM	85							

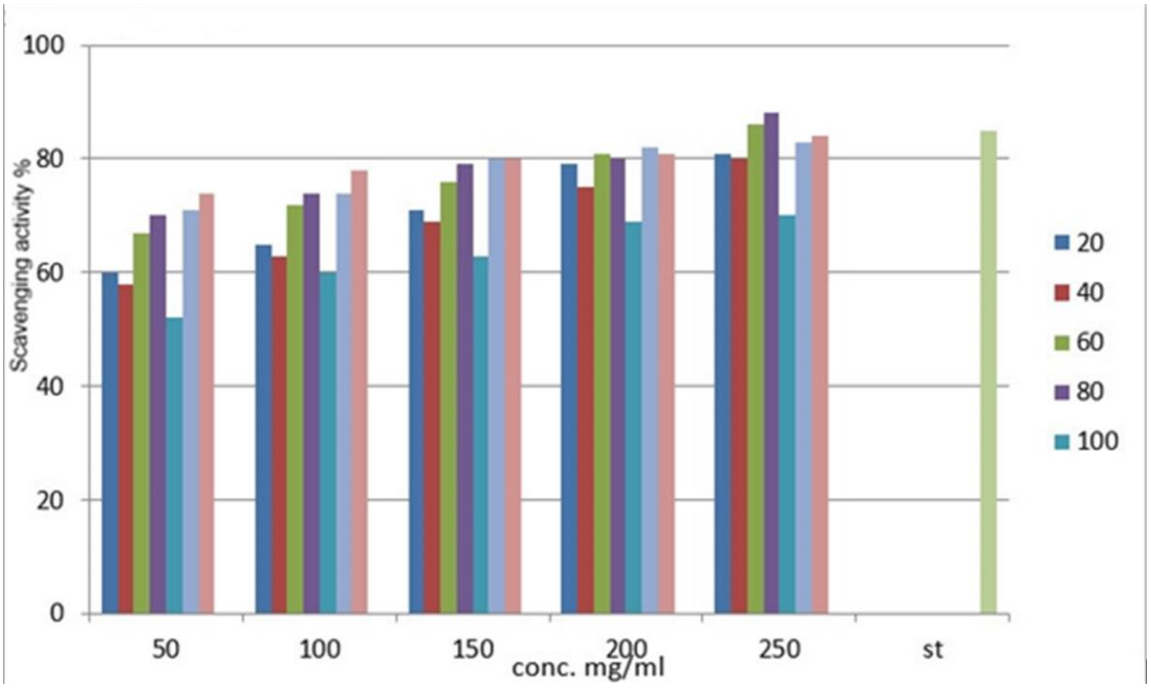

Figure 21. The scavenging activity of Imidazolidin-4-one derivatives G_1-G_8 compared to the reference standard vitamin C, as measured by the DPPH assay.

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4.Conclusion

This study provides key molecular insights that can be utilized to assess the antibacterial and antifungal activities of the Imidazolin-4-one ring and enhance its antioxidant properties.

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Author contributions The manuscript was prepared with contributions from all authors. All authors have approved the final version of the manuscript.

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Data availability No datasets were generated or analyzed during the current study. Declarations
.**Ethical approval** Not applicable
Competing interests The authors declare no competing interests

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