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Egypt. J. Chem. **58**, No. 6, pp. 645-657 (2015)

Uses of Isothiocyanate as Building Block in Syntheses of Triazole, Thiadiazole, Quinazoline, and Pyrimidine Systems of Agrochemical and Biological Activities

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DIFFERENT nitrogen heterocyclic compounds were synthesized in one pot reaction from 2-cyano-3-(4-hydroxy-3-methoxyphenyl) acryloyl isothiocyanate (2) as building block. The structures of the newly synthesized compounds were confirmed on the basis of their elemental and spectral analyses. The effect of the synthesized compounds on the growth of *Hordeum* coleoptile section using straight growth test for auxins and inhibitors has been studied. Moreover, some of the synthesized compounds were screened for their *in vitro* antibacterial activity against *Bacillus cereus* (Gram-positive bacteria), *Salmonella* (Gram negative bacteria) and antifungal activity against *Aspergillus niger.*

Keywords: Acryloyl isothiocyannate, Agro chemical activity and Antimicrobial activity .

Among the wide variety of heterocycles, pyrimidinone/thione and their derivatives have occupied an important position in natural and synthetic organic chemistry due to their wide range of biological activities, such as antioxidant, anti-inflammatory, anthelmintic, antimicrobial [1-3]. Pyrimidines have shown excellent broad spectrum herbicidal activity in transplanted paddy rice [4] , agro chemical fungicides [5,6] and exhibit remarkable activity as rubella virus inhibitors [7,8].

In addition, compounds incorporating substituted 1,2,4-triazole and 1,3,4-thiadiazole rings have been attracting widespread attention due to their diverse pharmacological properties such as antimicrobial, anti-inflammatory, analgesic and antitumor activities [9-12] .

Moreover, Quinazolinones have a diverse range of biological activities such as antibacterial, antifungal, analgesic, anti-inflammatory, cytotoxicity and diuretic [13-16] .

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In the process of searching for new active compounds, a number of heterocyclic systems carrying substituent (4-hydroxy-3-methoxyphenyl) as well as a cyano group and a thione have been synthesized. Therefore, our synthetic strategy is to synthesize heterocyclic systems using 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2) as building block. The synthesized compounds were screened for their antibacterial, antifungal activities and their effect on the growth of *Hordeum* coleoptile section.

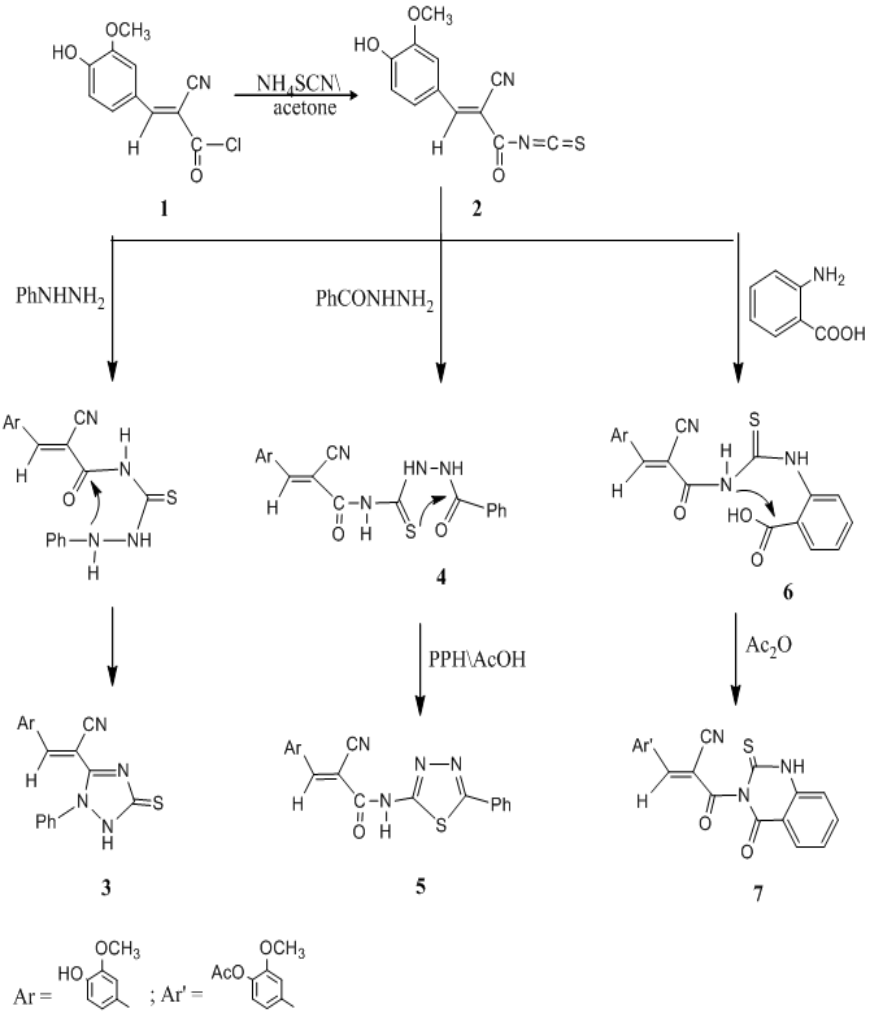
Results and Discussion

Chemistry

Biologically active heterocyclic compounds containing thione groups were synthesized in one pot reaction starting from 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2). Unstable acryloyl isothiocyanate derivative (2) was prepared *in situe* in the following reactions from the reaction of acid chloride (1) with ammonium thiocyanate in dry acetone. Triazole derivative (3) was prepared from the reaction of phenyl hydrazine with isothiocyanate (2) the reaction proceeds via addition of phenyl hydrazine to the isothiocyanate followed by exo-trig cyclization (Scheme 1). The structure of compound 3 was confirmed on the basis of its analytical and spectral data. The IR spectrum showed the absence of γ C=O band beside the presence of signals corresponding to γ NH (3390 cm^{-1}), γ CN (2280 cm^{-1}) and γ C=S (1388 cm^{-1}), respectively which supports the formation of 3. Moreover, the ^{1}H NMR spectrum revealed the presence of three singlets at δ 3.83, 7.98, 10.2 ppm corresponding to the OCH_3, CH=C— and OH protons (D_2O exchangeable), respectively beside the multiplet at δ 6.93–7.62 ppm for 8 aromatic protons and one NH proved the formation of triazole ring.

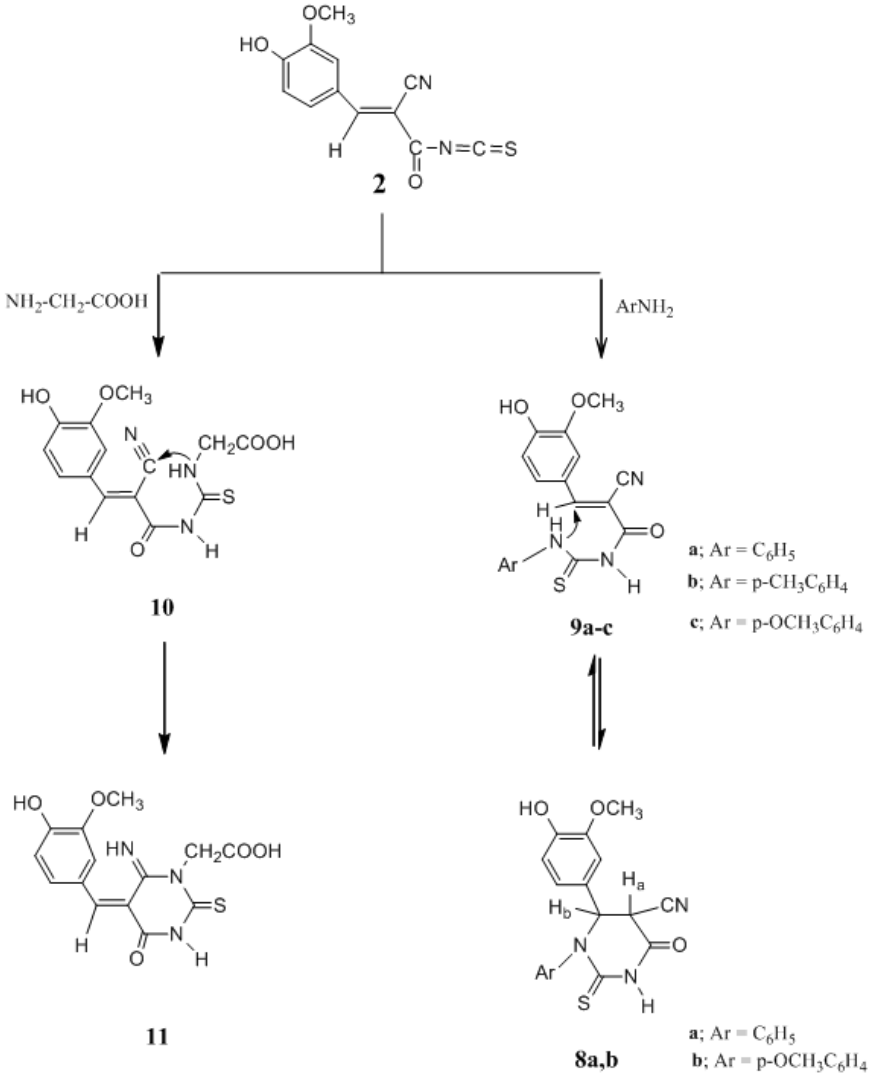
Addition of benzoyl hydrazine to isothiocyanate (2) afforded the benzoylhydrazinocarbonothioyl derivative (4) .Reaction of compound 4 with poly phosphoric acid in acetic acid involves the attack of the nucleophilic sulphur on the carbonyl group of the benzoyl moiety, followed by elimination of water molecule producing 1,3,4-thiadiazole derivative 5 (Scheme 1). The absence of thiocarbonyl γ C=S and γ C=O of the benzoyl moiety in the IR spectrum, beside the presence of only one NH in the ^{1}H NMR spectrum confirmed the formation of thiadiazole ring.

Moreover, when the isothiocyanate (2) reacts with anthranilic acid, acryloyl(thioureido)benzoic acid derivative (6) was obtained. Cyclization of 6 using acetic anhydride gave the 1,2-dihydroquinazoline derivative (7) (Scheme 1). The structure of 7 was confirmed on the basis of its analytical and spectral data (see the experimental section).



Scheme 1. Synthesis of compounds 3-7.

Reaction of isothiocyanate (2) with aromatic amines namely; aniline, p-toluidine and p-anisidine, gives different products depending upon the amine. In case of aniline, the product was hexahydropyrimidine derivative (8a). On the other hand, the reaction of 2 with p-toluidine afforded the thiourea derivative (9b). While, when the isothiocyanate 2 was treated with p-anisidine, the product was an equilibrium mixture of the thiourea derivative (9c) and the pyrimidine derivative (8b) (Scheme 2).



Scheme 2. Synthesis of compounds 8a, 9b, 8b ⇌ 9c and 11.

The reaction proceeds through the addition of amines to the isothiocyanate (2) producing the thiourea derivative intermediate (9a-c) which cyclize (in case of 8a) via Aza Micahel[17] addition of the NH on the olifinic bond (HC= C–) of the acryloyl moiety forming the pyrimidine derivative (8a). The structure of compounds 8a,b and 9a-c was confirmed on the basis of their analytical and spectral data. Therefore, ^{1}H NMR spectrum of compound 8a showed the presence of two singlets at δ 12.1 and 9.2 ppm (D_2O exchangeable) due to the presence of OH and NH groups, beside another singlet at δ 3.7 ppm for (OCH_3).

The presence of three doublets at 5.2, 5.4 and 5.7 ppm due to coupling between H_a and H_b, beside the absence of signal corresponding to the HC=C– (olefinic proton) prove the formation of hexahydropyrimidine ring. While, in case of p-anisidine, the presence of signals at 9.2 (NH), 8.2 (HC= C–) as well as the three doublets at 5.62, 5.35 and 5.14 ppm all of them integrating for two protons proved contribution of the structures 8b and 9c in equilibrium [18-20].

On the other hand, reaction of isothiocyanate 2 with glycine gives hexahydropyrimidine derivative 11 (Scheme 2). The reaction takes place via the intermediate formation of the acryloyl((thioureido)acetic acid derivative 10 which undergoes exo-dig cyclization via nucleophilic addition of NH on the cyano group of the acryloyl moiety. The IR spectrum of 11 showed the absence of γ CN band beside the presence of broad γ OH at 3600–3100 cm^{-1} and two bands at γ 1810, γ 1770 cm^{-1} for 2CO of cyclic amide and aliphatic acid, respectively which supports the formation of final product. Moreover, the presence of singlets at δ 3.98 ppm for the imino group (–C=NH, D_2O exchangeable), 4.67 ppm (CH_2), 7.94 ppm (HC=C–) in addition to two singlets at δ 10.54, 11.33 ppm for two hydroxyl groups (D_2O exchangeable) in the ^1H NMR spectrum proved the formation of imino pyrimidine structure.

Biological activity

Effect on the growth of Hordeum coleoptile sections

In this work, a number of heterocyclic systems carrying, in addition to the ring, other substituent (4-hydroxy-3-methoxy phenyl) as well as a cyano group and a thione. These rings are thought to have biological activity and this is why in this section, we have selected compounds (3, 8a, 9b, 8b ⇌ 9c) and we have studied their effect on the growth test for auxins and inhibitors[21].The obtained results are given in Table 1 and represented graphically in Fig. 1 and 2. The graph gives the variation of the length of coleoptile sections as percentage of control (in water) against concentration in ppm.

In all studied compounds, it was found that the relative high concentrations (10^3 and 10^2) inhibited the growth of *Hordeum* coleoptile sections, while the relative lower concentrations of all compounds studied, except the thiourea derivative (9b) stimulated this growth as being compared with the control (water). The optimum concentrations for growth stimulation was found to be 10^{-2} for triazoline thione (3) and 10^{-3} for pyrimidine thione (8a, 8b ⇌ 9c).

TABLE 1. Growth of *Hordeum* coleoptile sections as affected by different concentration.

Concentration (ppm)	Mean length of coleoptile sections as % of control			
	Compound (3)	Compound 8a	Compound 9b	Compound 8b ⇌ 9c
0.0 (control)	100	100	100	100
10^{3}	85	86	81	83
10^{2}	93	93	90	93
10^{1}	100	100	97	97
10^{0}	103	102	96	100
10^{-1}	101	103	98	103
10^{-2}	112	105	103	105
10^{-3}	106	106	100	107
10^{-4}	106	103	100	107
10^{-5}	105	102	100	100
10^{-6}	105	101	100	99.3

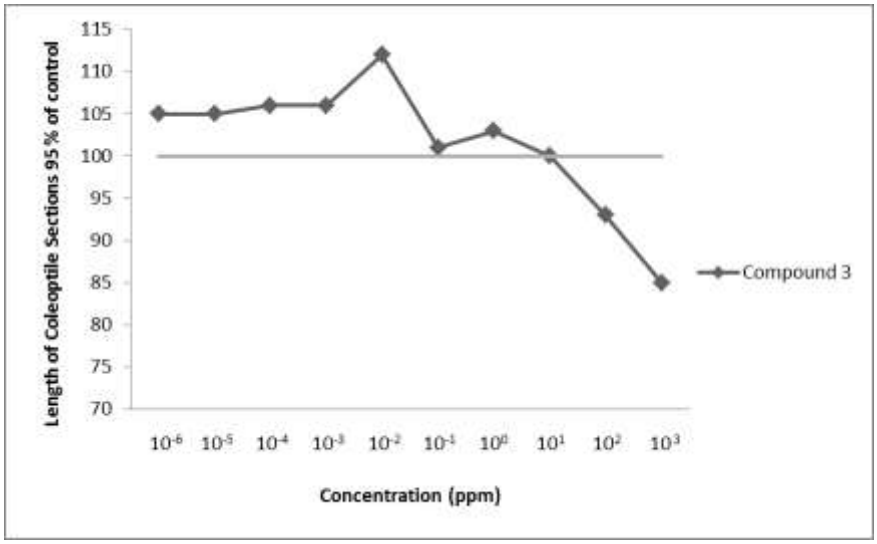


Fig. 1. Effect of compound 3 on the growth of *Hordeum* coleoptile sections .

The above results indicate that the compounds under investigation are biologically active and may be of hormonal nature.

In vitro antimicrobial activity

The synthesized compounds 3, 7, 8a, 9b and 8b 9c were tested for their antibacterial activity against two test organisms, *Bacillus cereus* (gram positive bacteria), *Salmonela* (gram negative bacteria) using the agar well-diffusion method[22] for studying the potential activities of these compounds using rifampicin (5 µg/disc) and ampicillin (10 µg/disc) as standard drugs.

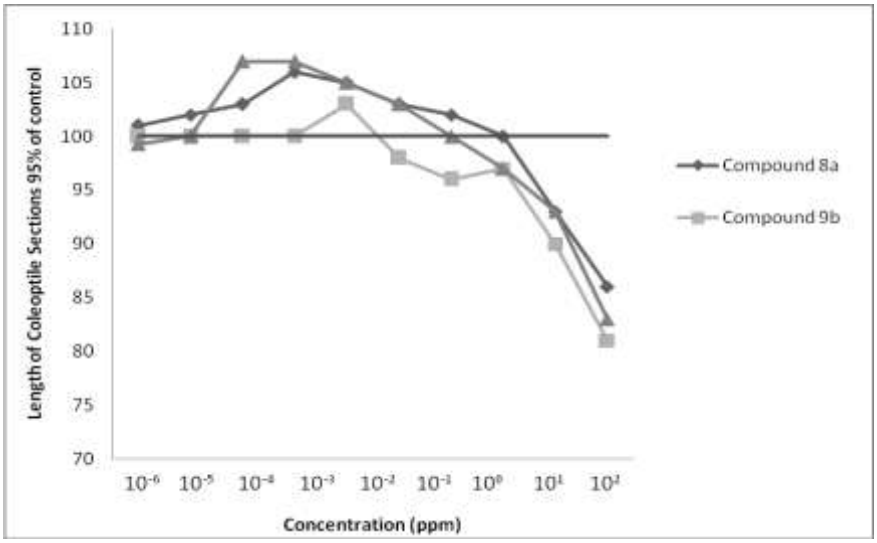


Fig. 2. Effect of compounds 8a, 9b and 8b ⇌9c on the growth of Hordeum coleoptile sections.

The antifungal activity of the synthesized compounds was tested against *Aspergillus niger* by a filter paper disc technique[23]. It was found that all tested compounds showed no significant effect against *Salmonela and Aspergillus niger*, whereas compounds 7, 9b and 8b 9c were active against *Bacillus cereus.* Minimum inhibitory concentration (MIC) values for the active compounds that showed inhibition zones > 10 mm were determined by means of the agar well-diffusion method in DMSO. The trend of activity was observed as follows: pyrimidine tautomer 8b 9c > Thio urea 9b > quinazoline derivative 7. The activity results of the synthesized compounds against *Bacillus cereus* shown in Table 2 as zone of inhibition (in mm) and minimum inhibitory concentration, MIC (mg/ml).

Conclusions

In this study, different nitrogen heterocyclic compounds were prepared in one pot reaction from 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2) through its reaction with different reagents. The effect of the synthesized compounds on the growth of *Hordeum* coleoptile section using straight growth test for auxins and inhibitors has been studied. The screening result showed that the relative high concentrations (10^3 and 10^2) inhibited the growth of *Hordeum* coleoptile sections. Moreover, the synthesized compounds 3, 7, 8a, 9b and 8b 9c were tested for their antibacterial activity against two test organisms, *Bacillus cereus, Salmonela* and antifungal activity against *Aspergillus niger.* It was found that, compounds 7, 9b and 8b 9c were active against *Bacillus cereus.*

TABLE 2. Determination of zone of inhibition and minimum inhibitory concentrations (MIC).

Compound No.	Zone of Inhibition (mm)	Minimum Inhibitory Concentration (MIC) mg/ml
	***Bacillus* cereus**	***Bacillus* cereus**
3	-	-
7	18	0.063
8a	-	
9b	19	0.063
8b 9c	22	0.05
Rifampicin	32	-
Ampicillin 3	30	-
DMSO	-	-

(-): No activity.

Experimental

All melting points were determined on a Stuart apparatus and the values given are uncorrected. IR spectra were determined on a Unicam SP 2000 using KBr, Wafer techniques and Mattson- 1000 FTIR spectrometer (Faculty of Science, Ain Shams University, Egypt). ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Varian Gemini 200, at 200 MHz and Varian EM-390 at 90 MHz spectrometer using TMS as the internal standard. Chemical shift values were recorded in ppm on δ scale. Mass spectra were recorded on a Shimadzu single focusing mass spectrometer at a beam energy 70 ev, where samples were introduced via a direct inlet system to the source; operating temperature at 250 °C (Microanalysis Center, Cairo University, Egypt). Elemental analyses were carried out by perkin-Elmer 2400.CHN, elemental analyser (Microanalysis Center, Cairo University, Egypt). The progress of the reactions was monitored using thin layer chromatography (TLC) sheets precoated with UV fluorescent silica gel Merck 60F 254 and were visualized using UV lamp

Synthesis of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl chloride (1)

A mixture of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acrylic acid.(2.19 g, 0.01 mol) (prepared from the saponification of ethyl 2-cyano-3-(4-hydroxy-3-methoxyphenyl(acrylate[24]) and thionyl chloride (50 ml) was heated under reflux on a boiling water bath for 2 hr. The excess thionyl chloride was distilled off, leaving a yellow product of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl chloride (1) Yield: 95%; m.p.: 125–127 °C; IR (KBr, cm^{-1}): 3400 (OH), 3048 (CH aromatic), 2220 (CN), 1750 (C=O).

Synthesis of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2)

When ammonium thiocyanate (0.76 g, 0.01 mol) was added to a solution of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl chloride (1) (2.37 g, 0.01 mol)

in dry acetone with stirring for 30 min, the reaction mixture was filtered off to get rid of ammonium chloride. The acetone solution contains 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2) was used for the following reactions.

Synthesis of 3-(4-hydroxy-3-methoxyphenyl)-2-(2-phenyl-5-thioxo-2,5-dihydro-1H-1,2,4-triazol-3-yl)acrylonitrile (3)

Phenyl hydrazine (1.08 g, 0.01 mol) was added to a solution of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2) (0.01 mol) prepared in *situ* in dry acetone. The reaction mixture was heated under reflux on a boiling water bath for 1 hr and the yellow product was precipitated, filtered off and crystallized from acetic acid.

Yield: 80 %; m.p.: 263–265 °C; IR (KBr, cm^{-1}): 3390 (NH), 2280 (CN), 1388 (C=S); ^{1}H NMR (DMSO-d_6): δ 3.83 (s, 3H, OCH_3), 6.93–7.62 (m, 9H, 8 Ar–H and 1 NH), 7.98 (s, 1H, HC=C—), 10.22 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 350 (M^+, 86.6). *Anal*. Calcd. for $C_{18}H_{14}N_4O_2S$: C, 61.7; H, 4.03; N, 15.99; S, 9.15. Found: C, 61.23; H, 3.86; N, 15.74; S, 8.95.

Synthesis of N-(2-benzoylhydrazinecarbonothioyl)-2-cyano-3-(4-hydroxy-3-methoxyphenyl)acrylamide (4)

Benzoyl hydrazine (1.36 g, 0.01 mol) was added to a solution of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2) (0.01 mol) prepared *in situ* in dry acetone. The reaction mixture was heated under reflux for 30 min. On evaporation of the excess acetone, a yellow product was precipitated, crystallized from toluene\ethanol mixture.

Yield: 83%; m.p.: 198–199 °C; IR (KBr, cm^{-1}): 3400-3260 (3NH), 2212 (CN), 1680, 1660 (2C=O), 1310 (C=S); ^{1}H NMR (DMSO-d_6): δ 3.81 (s, 3H, OCH_3), 7.01–7.62 (m, 9H, 8 Ar–H and 1 NH), 7.96 (s, 1H, HC=C–), 8.56 (s, 2H, NH, D_2O exchangeable), 10.54 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 396 (M^+, 55.7). *Anal*. Calcd. for $C_{19}H_{16}N_4O_4S$: C, 57.57; H, 4.07; N, 14.13; S, 8.09. Found: C, 57.83; H, 4.06; N, 13.8; S, 7.89.

Synthesis of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)-N-(5-phenyl-1,3,4-thiadiazol-2-yl)acrylamide (5)

When a solution of compound 4 (3.96 g, 0.01 mol) was heated under reflux with a mixture of polyphophoric acid (0.01 mol) in acetic acid (5 ml) for 2 hr, a yellow product was precipitated, filtered off, crystallized from acetic acid.

Yield: 75%; m.p.: 233–235 °C; IR (KBr, cm^{-1}): 3403 (NH), 2202 (CN), 1670 (C=O); ^{1}H NMR (DMSO-d_6): δ 3.79 (s, 3H, OCH_3), 7.12–7.73 (m, 8H, Ar–H), 7.94 (s, 1H, HC=C–), 8.56 (s, 1H, NH, D_2O exchangeable) 10.54 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 378 (M^+, 70.6). *Anal*. Calcd. for $C_{19}H_{14}N_4O_3S$: C, 60.31; H, 3.73; N, 14.81; S, 8.47. Found: C, 60.53; H, 3.96; N, 14.65; S, 8.23.

Synthesis of 2-(3-(2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl) thioureido) benzoic acid (6)

Anthranilic acid (1.37 g, 0.01 mol) was added to a solution of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2) (0.01 mol) prepared in *situ* in dry acetone. The reaction mixture was heated under reflux on a boiling water bath for 30 min. On evaporation of the excess acetone, a yellow product was precipitated and crystallized from acetic acid.

Yield: 75%; m.p.: 182–184 °C; IR (KBr, cm^{-1}): 3350-3260 (2NH), 2220 (CN), 1730, 1690 (2C=O), 1340 (C=S); ^{1}H NMR (DMSO-d_6): δ 3.78 (s, 3H, OCH_3), 6.98–7.59 (m, 7H, Ar–H), 7.97 (s, 1H, HC=C–), 8.61 (s, 2H, 2NH, D_2O exchangeable), 10.54 (s, 1H, OH, D_2O exchangeable), 11.33 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 397 (M^+, 15.4). *Anal*. Calcd. for $C_{19}H_{15}N_3O_5S$: C, 57.42; H, 3.80; N, 10.57; S, 8.07. Found: C, 57.13; H, 3.54; N, 10.34; S, 8.21.

Synthesis of 4-(2-cyano-3-oxo-3-(4-oxo-2-thioxo-1,2-dihydroquinazolin-3(4H)-yl)prop-1-en-1-yl)-2-methoxyphenyl acetate (7)

A solution of compound 6 (3.97 g, 0.01 mol) was heated under reflux with 10 ml acetic anhydride for 1.5 hr. The white product was precipitated, filtered off, crystallized from Toluene.

Yield: 60%; m.p.: 210–211 °C; IR (KBr, cm^{-1}): 3400 (NH), 2220 (CN), 1770, 1670, 1650 (3C=O), 1370 (C=S); ^{1}H NMR (DMSO-d_6): δ 2.39 (s, 3H, CH_3), 3.79 (s, 3H, OCH_3), 6.98–7.59 (m, 7H, Ar–H), 7.91 (s, 1H, HC=C–), 8.61 (s, 1H, NH, D_2O exchangeable); MS: *m/z* (%) 421 (M^+, 5.7). *Anal*. Calcd. for $C_{21}H_{15}N_3O_5S$: C, 59.85; H, 3.59; N, 9.97; S, 7.61. Found: C, 59.63; H, 3.54; N, 9.62; S, 7.45.

General procedure for the synthesis of 8a,b and 9a-c

Aromatic amines namely: aniline (0.93 g, 0.01mol), p-toluidine (1.07 g, 0.01 mol) and p-anisidine (1.23 g, 0.01 mol) were added to a solution of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)acryloyl isothiocyanate (2) (0.01 mol) prepared in *situ* in dry acetone. The reaction mixture was heated under reflux on a boiling water bath for 30 min and left to cool. On evaporation of the excess acetone, the yellow product was precipitated, filtered off and crystallized from toluene.

Synthesis of 6-(4-hydroxy-3-methoxyphenyl)-4-oxo-1-phenyl-2 thioxohexahydropyrimidine -5-carbonitrile (8a)

Yield: 75%; m.p.: 181–182 °C; IR (KBr, cm^{-1}): 3369 (NH), 2220 (CN), 1680 (C=O), 1370 (C=S); ^{1}H NMR (DMSO-d_6): δ 3.79 (s, 3H, OCH_3), 5.21, 5.43, 5.72 (3d, 2H, pyrimidine H_a and H_b) , 6.98–7.59 (m, 8H, Ar–H), 9.21 (s, 1H, NH, D_2O exchangeable) 12.14 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 353 (M^+, 2.9). *Anal*. Calcd. for $C_{18}H_{15}N_3O_3S$: C, 61.18; H, 4.28; N, 11.89; S, 9.07. Found: C, 61 .08; H, 4.06; N, 11.62; S, 9.25.

Synthesis of 2-cyano-3-(4-hydroxy-3-methoxyphenyl)-N-(p-tolylcarbamothioyl) acrylamide (9b)

Yield: 60%; m.p.: 189–190 °C; IR (KBr, cm^{-1}): 3390–3287 (2NH), 2220 (CN), 1680 (C=O), 1370 (C=S); ^{1}H NMR (DMSO-d_6): δ 2.35 (s, 3H, CH_3), 3.91 (s, 3H, OCH_3), 6.93–7.74 (m, 7H, Ar–H), 8.34 (s, 1H, HC=C–), 9.61 (s, 1H, NH, D_2O exchangeable), 10.54 (s, 1H, NH, D_2O exchangeable), 12.33 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 367 (M^+, 14.8). *Anal*. Calcd. for $C_{19}H_{17}N_3O_3S$: C, 62.11; H, 4.66; N, 11.44; S, 8.73. Found: C, 62.45; H, 4.54; N, 11.39; S, 8.65.

Synthesis of tautomeric mixture (8b ⇌ 9c)

Yield: 83%; m.p.: 190–191 °C; IR (KBr, cm^{-1}): 3387 (NH), 2210 (CN), 1690 (C=O), 1370 (C=S); ^{1}H NMR (DMSO-d_6): δ 3.79 (s, 3H, OCH_3), 3.88 (s, 3H, OCH_3), [5.62, 5.35, 5.14 (3dd, pyrimidine H_a and H_b of **8b** and 9.24 (NH), 8.21 (HC=C–) 2s, of **9c,** 2H], 6.98–7.59 (m, 7H, Ar–H), 10.51 (s, 1H, NH, D_2O exchangeable), 11.91 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 383 (M^+, 20.6). *Anal*. Calcd. for $C_{19}H_{17}N_3O_4S$: C, 59.52; H, 4.47; N, 10.96; S, 8.36. Found: C, 59.34; H, 4.20; N, 11.12; S, 8.25.

Synthesis of 2 - (5 - (4 – hydroxy – 3 – methoxybenzylidene)- 6 –imino -4-oxo-2-thioxotetrahydropyrimidin-1(2H)-yl)acetic acid (11)

Glycine (0.71 g, 0.01 mol) was added to a solution of acryloyl isothiocyanate (2) (0.01 mol) prepared in *situ* in dry acetone. The reaction mixture was heated under reflux on a boiling water bath for 1.5 hr. On evaporation of the excess acetone, a solid product was precipitated, washed with cold water to get rid of unreacted glycine and crystallized from toluene.

Yield: 55%; m.p.: 174–175 °C; IR (KBr, cm^{-1}): 3600–3200 (br. OH), 1810, 1770 (2C=O), 1370 (C=S); ^{1}H NMR (DMSO–d_6): δ 3.77 (s, 3H, OCH_3), 3.98 (s, 1H, –C=NH, D_2O exchangeable), 4.67 (s, 2H, CH_2), 6.98–7.31 (m, 3H, Ar–H), 7.94 (s, 1H, HC=C–), 8.41 (s, 1H, NH, D_2O exchangeable) 10.54 (s, 1H, OH, D_2O exchangeable), 11.33 (s, 1H, OH, D_2O exchangeable); MS: *m/z* (%) 335 (M^+, 5.7). *Anal*. Calcd. for $C_{14}H_{13}N_3O_5S$: C, 50.14; H, 3.91; N, 12.53; S, 9.56. Found: C, 50.33; H, 3.72; N, 12.34; S, 9.31.

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(*Received* 13/9/2015;
accepted 21/9/ 2015)

إستخدام الايزوثيوسيانات كمركب اساسى فى تحضيرمركبات الترىازول، ثيازول، كوينولين و بيريميدين ذات نشاط زراعى و بيولوجى

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فى هذا البحث تم تحضير مركبات مختلفة غير متجانسة الحلقة تحتوى على النيتروجين بإستخدام 2-سيانو-3-(4-هيدروكسى-3-ميثوكسى فينيل)اكريلويل أيزوثيوسيانات (2) كمركب اساسى. تم التعرف على التركيب الكيميائى لكل المركبات الجديدة المحضرة باستخدام الطرق الطيفية المختلفة وكذلك التحاليل الدقيقة لكل من الكربون، الهيدروجين، النيتروجين و الكبريت. كما تم دراسة تأثير المركبات المحضرة على نمو مقطع البراعم من نبات االشعير بأستخدام إختبار النمو المتساوى لكل من الاوكزين والمثبطات. كما تم الدراسة فى المعمل لتأثيربعض المركبات المحضرة على البكتريا موجبة الجرام (باسيلس سيريس) و البكتريا سالبة الجرام (سالمونيلا) وكذلك الفطريات (اسبرجيلاس نيجر)