



Synthesis, characterization and spectral studies of new pyrimidine compound

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ABSTRACT

A new series of some 3-{4-[6-(substituted phenyl)-2-thioxo-1,2,5,6-tetrahydro pyrimidin-4-yl] phenyl}-6-iodo-2-thioxo-2,3-dihydroquinazolin-4-one have been synthesized by reacting of 3-{4-[3-(substituted phenyl) prop-2-enoyl]phenyl}-6-iodo-2-thioxo-2,3-dihydroquinazolin-4-one (0.01M) with thiourea (0.01M) and 1g. of potassium hydroxide (KOH) in 30 ml of ethanol was refluxed for 3 hours. After syntheses compounds were characterized by chemical as well as instrumental methods. like elemental, IR and NMR. .

Key-words: quinazolin-4-one, thiourea, ethanol, IR, NMR..

INTRODUCTION

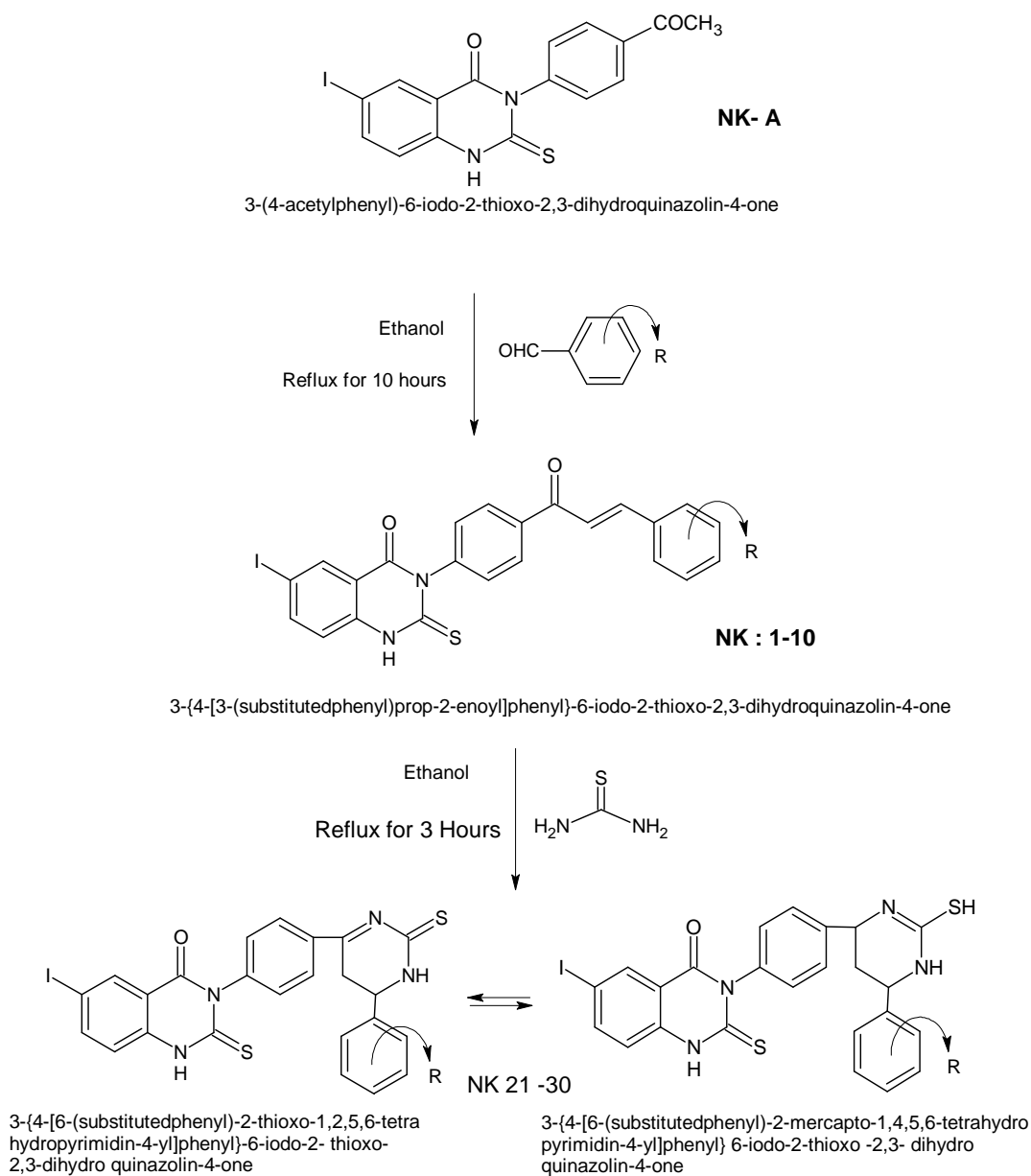
In recent years there has been an increasing interest in the chemistry of 4-quinazolinones because of their biological significance. Many of them show antifungal, antibacterial, anticancer, anti-inflammatory, anticonvulsant, immunotropic, hypolipidemic, antitumor, antiulcer and analgesic[1-13].

From the literature, we found that several quinazolinone derivatives are known to display antimicrobial and therapeutic actives. Literature survey reveals scant mention of the above compounds with antimicrobial properties and hence more and more derivatives are worth tested for the possible medicinal applications. So we have decided to synthesis 3-{4-[6-(substituted phenyl)-2-thioxo-1,2,5,6-tetrahydro pyrimidin-4-yl] phenyl}-6-iodo-2-thioxo-2,3-dihydroquinazolin-4-one

EXPERIMENTAL SECTION

All reagents were of analytical reagent grade and were used without further purification. All the product were synthesized and characterized by their spectral analysis, Chemicals Sodium Hydroxide, Hydrochloric acid, potassium hydroxide, thiourea and various aldehyde were purchased from S.D.fine chemicals (india).

Melting points were taken in open capillary tube. IR spectra were recorded on Shimadzu-PerkinElmer F.T I.R. Spectrophotometer Gx and Brooker instrument used for NMR Spectroscopy was 500 MHz and tetramethylsilane used as internal standard. Solvent used were DMSO. Purity of the compounds were checked by TLC on silica- G plates.

Reaction Scheme**Step: I Preparation of 3-{4-[3-(substituted phenyl) prop-2-enoyl] phenyl}-6-iodo-2-thioxo-2,3-dihydroquinazolin-4-one (NK:1-10).**

The solution of 3-(4-acetylphenyl)-6-iodo-2-thioxo-2,3-dihydroquinazolin-4-one (0.01M) in absolute ethanol (50 ml), substituted benzaldehyde (0.01M) and 2% NaOH (10 ml) were added and refluxed for 10 hours. After refluxing the reaction mixture was concentrated, cooled, filtered and neutralized with dil. HCl. The solid residue thus obtained was crystallized by absolute ethanol.

IR (KBr); NK-07 (cm⁻¹): 3420(>N-H of sec. amine), 3340(-OH), 3060(C-H, aromatic), 1690(>C=O), 1580(>C=C<, aromatic ring), 1240(>C=S), 1300(C-N), 1150(-C-O-), 510(C-I). **¹H NMR (DMSO) :** **NK-10 :** 3.78, singlet (1H) (-NH-), 7.76, Doublet (2H) (-CH=CH-Ar), 6.84-8.31, multiplet (11H) (Ar-H)

Step: II Preparation of 3-{4-[6-(substituted phenyl)-2-thioxo-1,2,5,6-tetrahydro pyrimidin-4-yl] phenyl}-6-iodo-2-thioxo-2,3-dihydroquinazolin-4-one (NK-21-30).

A mixture of 3-{4-[3-(substituted phenyl) prop-2-enoyl] phenyl} -6-iodo-2-thioxo-2,3-dihydroquinazolin-4-one (0.01M), thiourea (0.01M) and 1g. of potassium hydroxide(KOH) in 30ml of ethanol was refluxed for 3 hours. After standing overnight the solid formed was collected and crystallized from acetone.

IR (KBr); NK-21 (cm⁻¹): 3500(>N-H of sec. amine), 3020(=CH-), 1690(>C=O), 1600(>C=N), 1580(>C=C<, aromatic ring), 1470 (-CH₂), 1300(-C-N), 1240(>C=S), 680(C-Cl), 500(C-I).

¹H NMR (DMSO): NK-24: 1.88, Doublet (2H) (-CH₂-), 2.51, Doublet (1H) (-NH-), 3.76, Singlet (9H) (-OCH₃), 3.87, Triplet (1H) (-CH<), 4.11, Singlet (1H) (-NH-) 6.41-8.21, multiplet (9H) (Ar-H).

Table : 1 Physical constant of 3-{4-[6-(substituted phenyl)-2-thioxo-1,2,5,6-tetrahydro pyrimidin-4-yl] phenyl}-6-iodo- 2-thioxo-2,3-dihydroquinazolin-4-one

No.	Sub No.	R	Molecular Formula	Mol. Wt. (gm)	Yield (%)	M.P. \C	Carbon(%)		Hydrogen(%)		Nitrogen(%)	
							Found	required	Found	required	Found	required
1	NK-21	- 4-Cl	C ₂₄ H ₁₆ ClIN ₄ O ₂ S ₂	602.89	65	264	47.76	47.81	2.61	2.67	9.25	9.29
2	NK-22	- 2-Cl	C ₂₄ H ₁₆ ClIN ₄ O ₂ S ₂	602.89	68	252	47.76	47.81	2.61	2.67	9.25	9.29
3	NK-23	- 3,4-OCH ₃	C ₂₆ H ₂₁ IN ₄ O ₃ S ₂	628.50	72	262	49.65	49.69	3.31	3.37	8.87	8.91
4	NK-24	- 3,4,5-(OCH ₃) ₃	C ₂₇ H ₂₃ IN ₄ O ₄ S ₂	658.53	75	286	49.18	49.24	3.47	3.52	8.48	8.51
5	NK-25	- 2- OH	C ₂₄ H ₁₇ IN ₄ O ₂ S ₂	584.45	65	255	49.28	49.32	2.86	2.93	9.55	9.59
6	NK-26	- 4-OH , -3-OCH ₃	C ₂₅ H ₁₉ IN ₄ O ₃ S ₂	614.48	68	194	48.80	48.87	3.08	3.12	9.09	9.12
7	NK-27	- 4-OH	C ₂₄ H ₁₇ IN ₄ O ₂ S ₂	584.45	67	280	49.28	49.32	2.86	2.93	9.55	9.59
8	NK-28	- 4-N(CH ₃) ₂	C ₂₆ H ₂₂ IN ₅ O ₂ S ₂	611.52	68	253	51.03	51.07	3.55	3.63	11.41	11.45
9	NK-29	- 4-OCH ₃	C ₂₅ H ₁₉ IN ₄ O ₂ S ₂	598.48	69	282	50.13	50.17	3.15	3.20	9.32	9.36
10	NK-30	- 3- NO ₂	C ₂₄ H ₁₆ IN ₃ O ₃ S ₂	613.45	62	230	46.92	46.99	2.60	2.63	11.38	11.42

Acknowledgements

The authors are thankful to the M.N. College, Visnagar for providing research facilities.

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