

# Synthesis of Some New Quinazoline Derivatives and Theoretical Studies of their Geometries

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## Abstract

Quinazoline and their fused-ring systems are well known for their potential biological activity. Inspired by this and in view of the usefulness of heterocyclic thiols as vulcanization accelerators, new derivatives viz. Quinazoline-2-thiols were prepared. These were synthesized by the condensation of 2-[isothiocyanato(substituted phenyl)methyl]-3,4-dihydronaphthalene-1(2H)-one with primary aromatic amines. All the prepared compounds have been characterized by elemental analysis, IR and mass spectroscopy.

**Keywords:** Quinazoline; Quinazoline-2-thiols; Fused-ring systems; Condensation.

## 1. Introduction

In the family of heterocyclic compounds, nitrogen-containing heterocycles are an important class of compounds in medicinal chemistry. There has been considerable interest in the development of preparative methods for the production of quinazolines [1]. This is because quinazolines and their ring-fused derivatives display a broad spectrum of biological activities [2] like anti-tubercular, analgesic, anti-inflammatory, and anti-bacterial. Adding to this class of heterocyclic compounds, we have reported earlier [3] the reaction of aromatic aldehyde, thiourea and cyclic ketone to synthesize quinazoline-2(1H)-thiones. Then, these were alkylated/aralkylated. The present paper describes the reaction of 2-[isothiocyanato(substituted phenyl)methyl]-3,4-dihydronaphthalene-1(2H)ones with primary aromatic amines to give another cyclized products viz. quinazoline-2-thiols. Our literature survey reveals that quinazoline-2-thiols are unknown in the literature except for a report mentioning the synthesis of similar compounds [4, 5] 1-(substituted phenyl)-4,4,6-trimethyl-1H,4H-pyrimidine-2-thiols. The later compounds have shown many biological activities [6-8] like anticonvulsive activity like a well-known drug phenobarbitone, as the structure of both of these, are somewhat chemically similar. Also, it has been mentioned in the literature that heterocyclic thiols can act as vulcanization accelerators [4]. Therefore, working on the similar guidelines and in continuation with our research program dealing with the synthesis of biologically active compounds, we report herein a general route to the title compounds.

## 2. Methods

Melting points were determined in open-end capillaries and are uncorrected. Compounds were checked for their purity by TLC on silica gel G plates and spots were located by iodine vapors. <sup>1</sup>H NMR spectra were recorded on BRUKER ADVANCE II 400 NMR Spectrometer using TMS as internal standard. The mass spectra were obtained on a JEOL 5x102/DA-6000 mass spectrometer. The IR spectra were recorded on Perkin-Elmer spectrum RX IFT-IR System using KBr pellets. Elemental analyses of the newly synthesized compounds were carried out on Perkin Elmer model 2400 C H N analyzer. All the compounds gave satisfactory elemental analysis within  $\pm 0.4\%$  of theoretical values. The microwave-irradiated reactions were performed in domestic household microwave oven Samsung M177N.

### General procedure for the synthesis of 2-arylidene-tetralin-1-one (1a-1i):

A mixture of  $\alpha$ -tetralone and substituted aromatic aldehydes were subjected to microwave heating for 2-5 minutes using absolute alcohol (5 ml) as energy transfer medium and conc. HCl (0.5 ml) as a catalyst. The reaction mixture was cooled to room temperature. The solid, so obtained, was filtered, washed with ethanol and finally crystallized from ethanol to give 1a-1i.

**Table 1:** Synthesis of 2-arylidene tetralin-1-one (1a-1i).

Product	R	Time (min)	Yield (%)	M.pt. (°C)	Lit.m.pt <sup>14-16</sup> (°C)	IR (KBr, cm <sup>-1</sup> )
1a	H	4.30	50	104-105	105,102-103	1661.2 (C=O), 1589.6(C=C), 1491.1 (C ≡ C)
1b	2,4(Cl)	2.30	35	54-56	----	----
1c	4-NO <sub>2</sub>	4.00	42	182-183	184,185	----
1d	3-NO <sub>2</sub>	4.00	38	142-143	----	----
1e	4-OCH <sub>3</sub>	4.15	40	109-110	110,109	----
1f	2,3(O-CH <sub>2</sub> -O)	4.30	75	133-139	----	----
1g	4-Br	4.00	47	158-159	----	----
1h	3-OH	4.00	37	135-139	----	----
1i	4-CH <sub>3</sub>	3.30	36	125-126	124	----

The PMR spectra of compound 1e shows a multiplet due to aromatic protons at  $\delta$  7.89-6.93. The triplets at  $\delta$  3.09-3.07 &  $\delta$  2.94-2.93 were assigned to C<sub>5</sub>CH<sub>2</sub> & C<sub>6</sub>CH<sub>2</sub>. A singlet was observed at  $\delta$  3.83 due to 4-OCH<sub>3</sub>. Also, a singlet was observed at  $\delta$  1.79 due to =CH proton.

#### General procedure for the synthesis of 2-[isothiocyanato(substituted phenyl)methyl]-3,4-dihydronaphthalene-1(2H)-one (2a-2i):

The mixture of compound 1a-1i (1 mole) and potassium isothiocyanate (1 mole) was taken in a conical flask. To it few pieces of ice were added and then H<sub>2</sub>SO<sub>4</sub> (9.8 ml, 1 mole) was added drop wise. It was stirred for 15-20 minutes. The solid product, so obtained, was washed with sodium carbonate and then with distilled water. The IR spectral values of some of the representative members are given below:

**Table 2:** Synthesis of 2-[isothiocyanato(substituted phenyl)methyl]-3,4-dihydronaphthalene-1(2H)-one (2a-2i).

Product	R	IR (KBr, cm <sup>-1</sup> ); PMR (ppm, $\delta$ )
2a	H	2056.1 (NCS); 1664.8 (C=O); 1454.7 (C ≡ C); 1223.7 (C-N)
2d	3-NO <sub>2</sub>	2050.3 (NCS); 1664.2 (C=O); 1529.3 (NO <sub>2</sub> ); 1224.4 (C-N)
2e	4-OCH <sub>3</sub>	2055.8 (NCS); 1645 (C=O); 1510 (C ≡ C); 1178.4 (C-N); 7.99-6.97 (m, 8H, Ar-H), 3.85 (s, 3H, 4-OCH <sub>3</sub> ), 3.09-3.07 (t, 2H, C <sub>5</sub> CH <sub>2</sub> or C <sub>6</sub> CH <sub>2</sub> ), 2.94-2.93 (t, 2H, C <sub>5</sub> CH <sub>2</sub> or C <sub>6</sub> CH <sub>2</sub> ), 1.81-1.80 (d, 1H, C <sub>2</sub> H), 1.42-1.35 (d, 1H, C <sub>1</sub> H)
2i	4-CH <sub>3</sub>	2057.9 (NCS); 1654.1 (C=O); 1516.4 (C ≡ C); 1313 (C-N)

#### Synthesis of 1-(substitutedphenyl)-4-aryl-1,4,5,6-tetrahydrobenzo[h]quinazoline-2-thiol (3-9):

A mixture of 2a-2i (0.01 mole), substituted anilines (0.01 mole) and ethanol (2-3 ml) was taken in a flask. To it, few drops (4-5) of H<sub>2</sub>SO<sub>4</sub> was added and stirred for 5-10 minutes. Solid separated was washed with glacial acetic acid and then with distilled water.

#### Characterization data of 1-(substitutedphenyl)-4-aryl-1,4,5,6-tetrahydrobenzo[h]quinazoline-2-thiol (3-9):

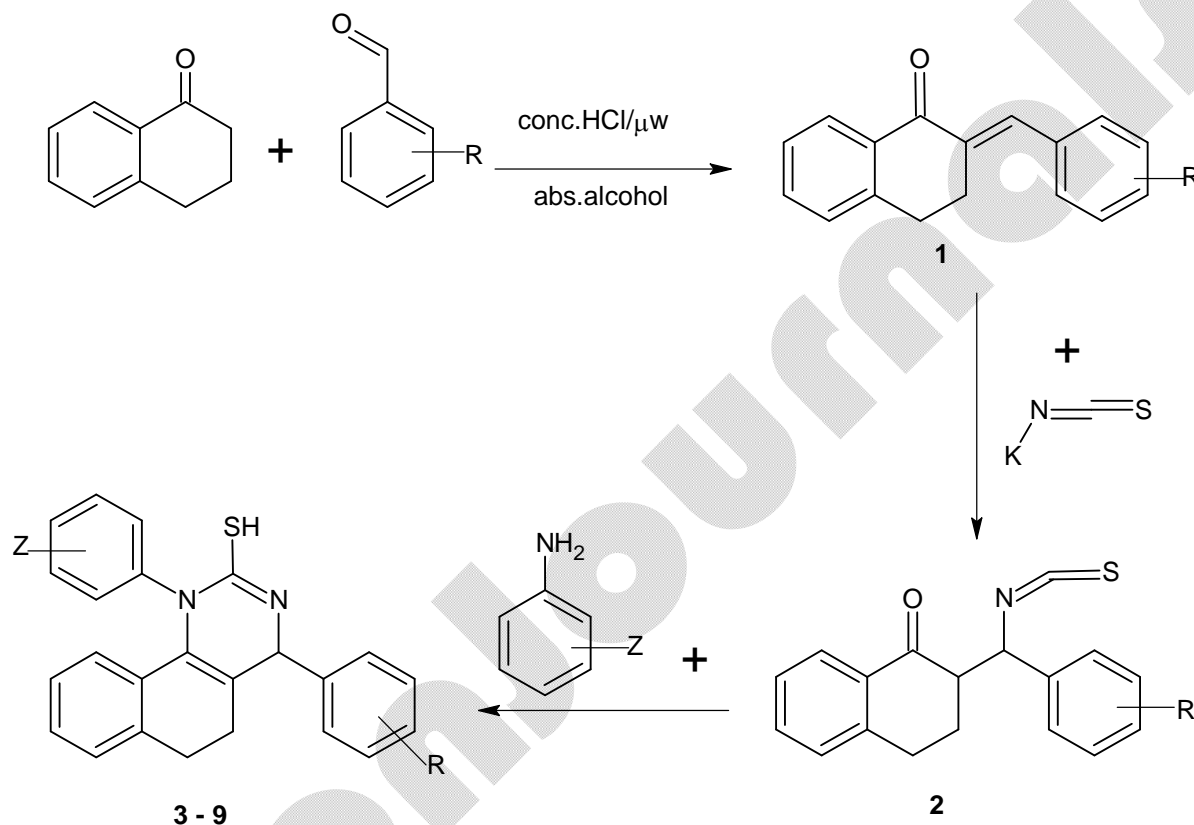
Product	Z	R	Yield; IR (KBr, cm <sup>-1</sup> ); Mass(m/z); Elemental analysis, <sup>1</sup> H ( $\delta$ , ppm)
3a	2-CH <sub>3</sub>	H	76%; 217-219; 2850.4 (arom. C-H str.), 2604.7 (S-H), 1637 (C=N), 1560 (C=C), 1498.4 (C ≡ C); 1313.9 (C-N) 382.10 M <sup>+</sup> (60.79%), 218.15 (97.04%), 128.05 (3.07%), 105.90 (100%), 90.15 (4.36%), 77 (28.65%), 65.05 (6.61%), 50.05 (5.55%) Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> S: C 78.53; H 5.76; N 7.33. Found: C 78.45; H 5.62; N 7.21%
3b	2-CH <sub>3</sub>	2,4(Cl)	40%; 215-217; Anal. Calcd. For C <sub>25</sub> H <sub>20</sub> N <sub>2</sub> S: C 66.66; H 4.44; N 6.22. Found: C 66.56; H 4.38; N 6.15%
3c	2-CH <sub>3</sub>	4-NO <sub>2</sub>	77%; 223-225; Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>3</sub> SO <sub>2</sub> : C 70.26; H 4.92; N 9.84.

			Found: C 70.19; H 4.88; N 9.76%
3d	2-CH <sub>3</sub>	3-NO <sub>2</sub>	44%; 218-220; 2909.4 (arom. C-H str.), 2654.6 (S-H), 1616.9 (C=N), 1544.5 (C=C), 1495.2(C $\equiv$ C); 1394.4 (C-N) Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>3</sub> SO <sub>2</sub> : C 70.26; H 4.92; N 9.84. Found: C 70.22; H 4.86; N 9.80%
3e	2-CH <sub>3</sub>	4-OCH <sub>3</sub>	13%; 222-224; 2870.2 (arom. C-H str.), 2604.6 (S-H), 1640.4 (C=N), 1590 (C=C), 1461.9 (C $\equiv$ C); 1302 (C-N) 7.95 (s, 1H, SH), 7.66-6.78 (m, 12H, Ar-H), 4.80 (s, 1H, C <sub>4</sub> H), 3.74 (s, 3H, 4-OCH <sub>3</sub> ), 3.09-3.07 (t, 2H, C <sub>5</sub> CH <sub>2</sub> or C <sub>6</sub> CH <sub>2</sub> ), 2.94-2.93 (t, 2H, C <sub>5</sub> CH <sub>2</sub> or C <sub>6</sub> CH <sub>2</sub> ), 2.54-2.53 (s, 3H, 4-OCH <sub>3</sub> ), 2.21 (s, 3H, CH <sub>3</sub> )  Anal. Calcd. For C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> SO: C 75.72; H 5.82; N 6.79. Found: C 75.65; H 5.78; N 6.65%
3f	2-CH <sub>3</sub>	2,3(O-CH <sub>2</sub> -O)	85%; 215-219; 276 (1.75%), 122 (4.58%), 65 (5.88%), 63.95 (100%), 58.10 (0.60%), 52.10 (6.85%), 40.10 (2.54%) Anal. Calcd. For C <sub>26</sub> H <sub>22</sub> N <sub>2</sub> SO <sub>2</sub> : C 73.24; H 5.16; N 6.57. Found: C 73.16; H 5.20; N 6.42%
3g	2-CH <sub>3</sub>	4-Br	224-225; 2820 (arom. C-H str.), 2589 (S-H), 1601.9 (C=N), 1485.2 (C=N), 1400.2(C $\equiv$ C); 1317.5 (C-N) Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>2</sub> S: C 64.93; H 4.54; N 6.06. Found: C 64.99; H 4.42; N 6.01%
3h	2-CH <sub>3</sub>	3-OH	38%; 228-230; Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> SO: C 75.38; H 5.53; N 7.03. Found: C 75.29; H 5.47; N 6.95%
3i	2-CH <sub>3</sub>	4-CH <sub>3</sub>	38%; 222-224; 2910.4 (arom. C-H str.), 2655.3 (S-H), 1586.8 (C=N), 1544.8 (C=C), 1495(C $\equiv$ C); 1316.4 (C-N) Anal. Calcd. For C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> S: C 78.78; H 6.06; N 7.07. Found: C 78.69; H 5.99; N 7.01%
4a	4-CH <sub>3</sub>	H	69%; 239-241; Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> S: C 78.53; H 5.76; N 7.33. Found: C 78.49; H 5.66; N 7.25%
4b	4-CH <sub>3</sub>	2,4(Cl)	38%; 232-234; Anal. Calcd. For C <sub>25</sub> H <sub>20</sub> N <sub>2</sub> S: C 66.66; H 4.44; N 6.22. Found: C 66.59; H 4.37; N 6.17%
4c	4-CH <sub>3</sub>	4-NO <sub>2</sub>	69%; 216-218; Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>3</sub> SO <sub>2</sub> : C 70.26; H 4.92; N 9.84. Found: C 70.21; H 4.86; N 9.78%
4d	4-CH <sub>3</sub>	3-NO <sub>2</sub>	36%; 237-239; Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>3</sub> SO <sub>2</sub> : C 70.26; H 4.92; N 9.84. Found: C 70.20; H 4.95; N 9.78%
4e	4-CH <sub>3</sub>	4-OCH <sub>3</sub>	07%; 220-222; Anal. Calcd. For C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> SO: C 75.72; H 5.82; N 6.79. Found: C 75.68; H 5.75; N 6.83%
4f	4-CH <sub>3</sub>	2,3(O-CH <sub>2</sub> -O)	77%; 221-223; Anal. Calcd. For C <sub>26</sub> H <sub>22</sub> N <sub>2</sub> SO <sub>2</sub> : C 73.24; H 5.16; N 6.57. Found: C 73.29; H 5.11; N 6.49%
4g	4-CH <sub>3</sub>	4-Br	31%; 246-248; 2874.8 (arom. C-H str.), 2596.4 (S-H), 1592.2 (C=N), 1485.5 (C=C), 1400.1(C $\equiv$ C); 1297.9 (C-N) Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>2</sub> S: C 64.93; H 4.54; N 6.06. Found: C 64.89; H 4.46; N 5.97%
4h	4-CH <sub>3</sub>	3-OH	38%; 253-255; Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> SO: C 75.38; H 5.53; N 7.03. Found: C 75.43; H 5.48; N 6.99%
4i	4-CH <sub>3</sub>	4-CH <sub>3</sub>	38%; 235-237; 2924 and 2849 (arom. (C-H), 2590.9 (S-H), 1617.8 (C=N), 1559.8 (C=C), 1458.2(C $\equiv$ C); 1320.9 (C-N) 396, 277, 276, 128, 105, 103, 65, 58, 40 Anal. Calcd. For C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> S: C 78.78; H 6.06; N 7.07. Found: C 78.71; H 6.12; N 7.13%
5a	4-OCH <sub>3</sub>	H	71%; 246-249; 2918 (arom. C-H str.), 2603.4 (S-H), 1618.1 (C=N), 1513.5 (C=C), 1458.1(C $\equiv$ C); 1303 (C-N) Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> SO: C 75.37; H 5.53; N 7.03. Found: C 75.29; H 5.44; N 7.11%
5b	4-OCH <sub>3</sub>	2,4(Cl)	77%; 240-242; Anal. Calcd. For C <sub>25</sub> H <sub>20</sub> N <sub>2</sub> SO: C 64.38; H 4.29; N 6.01. Found: C 64.29; H 4.21; N 5.92%
5c	4-OCH <sub>3</sub>	4-NO <sub>2</sub>	90%; 241-243; Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>3</sub> SO <sub>2</sub> : C 67.72; H 4.74; N 9.48. Found: C 67.68; H 4.63; N 9.40%
5d	4-OCH <sub>3</sub>	3-NO <sub>2</sub>	34%; 238-240; Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>3</sub> SO <sub>2</sub> : C 67.72; H 4.74; N 9.48. Found: C 67.66; H 4.67; N 9.42%

5e	4-OCH <sub>3</sub>	4-OCH <sub>3</sub>	65%; 253-255; Anal. Calcd. For C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> SO <sub>2</sub> : C 72.89; H 5.61; N 6.54. Found: C 72.76; H 5.57; N 6.49 %
5f	4-OCH <sub>3</sub>	2,3(O-CH <sub>2</sub> -O)	78%; 247-249; Anal. Calcd. For C <sub>26</sub> H <sub>22</sub> N <sub>2</sub> SO <sub>3</sub> : C 70.59; H 4.98; N 6.33. Found: C 70.48; H 4.89; N 6.39 %
5g	4-OCH <sub>3</sub>	4-Br	254-255; Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>2</sub> SO: C 62.76; H 4.39; N 5.86. Found: C 62.69; H 4.30; N 5.74 %
5h	4-OCH <sub>3</sub>	3-OH	269-271; Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> SO <sub>2</sub> : C 72.46; H 5.31; N 6.76. Found: C 72.52; H 5.39; N 6.82 %
5i	4-OCH <sub>3</sub>	4-CH <sub>3</sub>	74%; 245-247; 2919.6 (arom. C-H str.), 2596.4 (S-H), 1600 (C=N), 1586.6 (C=C), 1453.6 (C $\equiv$ C); 1317.6 (C-N) Anal. Calcd. For C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> SO: C 75.73; H 5.82; N 6.79. Found: C 75.68; H 5.77; N 6.69 %
6a	4-Cl	H	71%; 242-244; Anal. Calcd. For C <sub>24</sub> H <sub>19</sub> N <sub>2</sub> S: C 71.64; H 4.73; N 6.96. Found: C 71.52; H 4.79; N 6.88 %
6b	4-Cl	2,4(Cl)	58%; 254-256; Anal. Calcd. For C <sub>24</sub> H <sub>17</sub> N <sub>2</sub> S: C 61.28; H 3.62; N 5.95. Found: C 61.23; H 3.68; N 5.89 %
6c	4-Cl	4-NO <sub>2</sub>	33%; 229-231; Anal. Calcd. For C <sub>24</sub> H <sub>18</sub> N <sub>3</sub> SO <sub>2</sub> : C 64.43; H 4.03; N 9.39. Found: C 64.47; H 4.09; N 9.25 %
6d	4-Cl	3-NO <sub>2</sub>	37%; 244-246; Anal. Calcd. For C <sub>24</sub> H <sub>18</sub> N <sub>3</sub> SO <sub>2</sub> : C 64.43; H 4.03; N 9.39. Found: C 64.39; H 4.11; N 9.29 %
6e	4-Cl	4-OCH <sub>3</sub>	10%; 235-237; Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>2</sub> SO: C 69.44; H 4.86; N 6.48. Found: C 69.47; H 4.78; N 6.32 %
6f	4-Cl	2,3(O-CH <sub>2</sub> -O)	79%; 240-242; Anal. Calcd. For C <sub>25</sub> H <sub>19</sub> N <sub>2</sub> SO <sub>2</sub> : C 67.26; H 4.26; N 6.28. Found: C 67.19; H 4.23; N 6.24 %
6g	4-Cl	4-Br	31%; 253-255; Anal. Calcd. For C <sub>24</sub> H <sub>18</sub> N <sub>2</sub> S: C 59.75; H 3.73; N 5.81. Found: C 59.67; H 3.65; N 5.72 %
6h	4-Cl	3-OH	37%; 264-266; Anal. Calcd. For C <sub>24</sub> H <sub>19</sub> N <sub>2</sub> SO: C 68.89; H 4.54; N 6.69. Found: C 68.80; H 4.42; N 6.58 %
6i	4-Cl	4-CH <sub>3</sub>	74%; 255-256; 2925.9 (arom. C-H str.), 2590 (S-H), 1617.2 (C=N), 1559.8 (C=C), 1494.2 (C $\equiv$ C); 1289.2 (C-N) 357, 229, 129, 128, 127, 125, 92, 65, 26 Anal. Calcd. For C <sub>25</sub> H <sub>21</sub> N <sub>2</sub> S: C 72.11; H 5.05; N 6.73. Found: C 72.02; H 5.12; N 6.65 %
7a	4-COOH	H	71%; 2911.7 (arom. C-H), 2596 (S-H), 1613.8 (C=N), 1513.8 (C=C), 1431.7 (C $\equiv$ C); 1394.5 (C-N) Anal. Calcd. For C <sub>25</sub> H <sub>20</sub> N <sub>2</sub> SO <sub>2</sub> : C 72.81; H 4.85; N 6.79. Found: C 72.72; H 4.93; N 6.68 %
7i	4-COOH	4-CH <sub>3</sub>	46%; 2919.5 (arom. C-H), 2603.9 (S-H), 1601.2 (C=N), 1586.6 (C=C), 1455.3 (C $\equiv$ C); 1317.7 (C-N) Anal. Calcd. For C <sub>26</sub> H <sub>22</sub> N <sub>2</sub> S: C 73.23; H 5.16; N 6.57. Found: C 73.15; H 5.12; N 6.65 %
7f	4-COOH	2,3(O-CH <sub>2</sub> -O)	71%; 230-232(d); 91 (2.01%), 65.05 (1.88%), 52.40 (1.50%), 43.90 (100%) Anal. Calcd. For C <sub>26</sub> H <sub>20</sub> N <sub>2</sub> SO <sub>4</sub> : C 68.42; H 4.38; N 6.14. Found: C 68.32; H 4.29; N 6.09 %
8a	H	H	2874.1 (arom. C-H), 2588.9 (S-H), 1600 (C=N), 1557.8 (C=C), 1494.3 (C $\equiv$ C); 1328.7 (C-N) Anal. Calcd. For C <sub>24</sub> H <sub>20</sub> N <sub>2</sub> S: C 78.26; H 5.55; N 7.61. Found: C 78.35; H 5.48; N 7.72 %
8e	H	4-OCH <sub>3</sub>	2871.6 (arom. C-H), 2589 (S-H), 1600.1 (C=N), 1494.6 (C=C), 1328.7 (C-N) Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> S: C 75.37; H 5.53; N 7.03. Found: C 75.28; H 5.43; N 7.24 %
8i	H	4-CH <sub>3</sub>	2590 (S-H), 1654.1 (C=N), 1508.3 (C=C) Anal. Calcd. For C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> S: C 78.53; H 5.76; N 7.33. Found: C 78.46; H 5.82; N 7.21 %
9i	2-NH <sub>2</sub>	4-CH <sub>3</sub>	3334 & 3412 (N-H), 2924 (arom. C-H), 2596.4 (S-H), 1577 (C=N), 1540.9 (C=C), 1463.8 (C $\equiv$ C); 1316.7 (C-N) 269, 176, 128, 127, 106, 92, 65, 59, 41 Anal. Calcd. For C <sub>25</sub> H <sub>23</sub> N <sub>3</sub> S: C 75.56; H 5.79; N 10.57. Found: C 75.67; H 5.70; N 10.46 %

### 3. Results and Discussion

2-Arylidene tetralin-1-one (**1**), obtained by the reaction of  $\alpha$ -tetralone and substituted aromatic aldehyde, when treated with potassium isothiocyanate gave 2-[isothiocyanato(substituted phenyl)methyl]-3,4-dihydronaphthalene-1(2*H*)-one (**2**). Infrared absorption spectra measurements of compounds 2a-2i showed a band at about  $2040\text{ cm}^{-1}$ , the characteristic broad band attributed to the isothiocyanato group. This compound on further reaction with primary aromatic amine gave 1-(substituted phenyl)-4-aryl-1,4,5,6-tetrahydrobenzo[*h*]quinazoline-2-thiol (**3-9**) (**Scheme 1**). The IR spectra of the prepared compounds displayed the characteristic S-H stretching vibration at  $2550\text{-}2600\text{ cm}^{-1}$ . In addition, the Mass Spectra (MS) of the compound 3a showed the molecular ion peak at 382 while the MS of maximum compounds did not show any molecular ion peak but showed the peaks due to fragments that supported the expected structure.

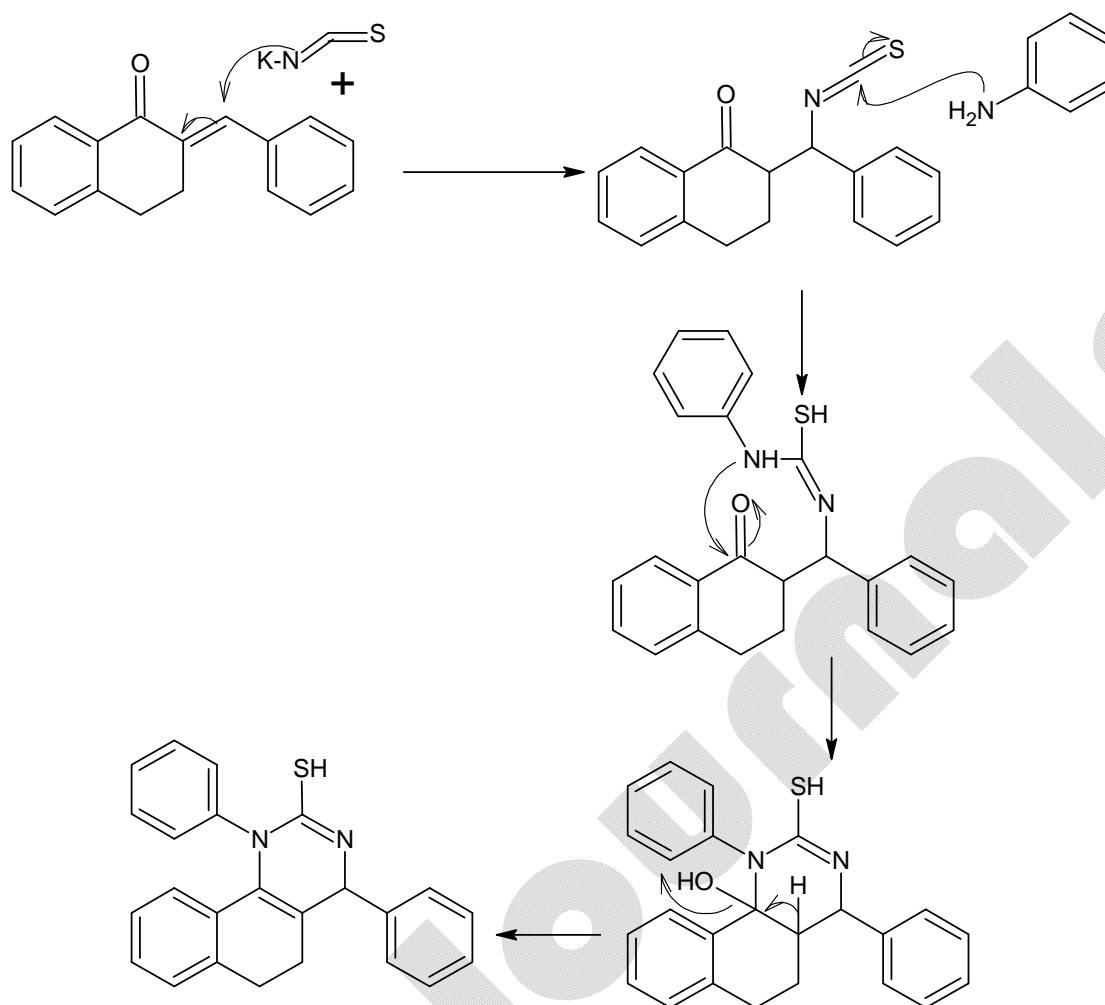


Z = (3) 2-CH<sub>3</sub> (4) 4-CH<sub>3</sub> (5) 4-OCH<sub>3</sub> (6) 4-Cl (7) 4-COOH (8) H (9) 2-NH<sub>2</sub>

R = (a) H (b) 2,4(Cl) (c) 4-NO<sub>2</sub> (d) 3-NO<sub>2</sub> (e) 4-OCH<sub>3</sub> (f) 2,3(O-CH<sub>2</sub>-O) (g) 4-Br (h) 3-OH (i) 4-CH<sub>3</sub>

Scheme 1

As an example, the disappearance of IR band for isothiocyanato group at  $2055.8\text{ cm}^{-1}$  and appearance of S-H band at  $2604.6\text{ cm}^{-1}$  clearly proves the formation of 3e from 2e. Therefore, the spectroscopic data along with the literature survey [4-5], helped in proposing the following **mechanism** for the above-mentioned reaction:

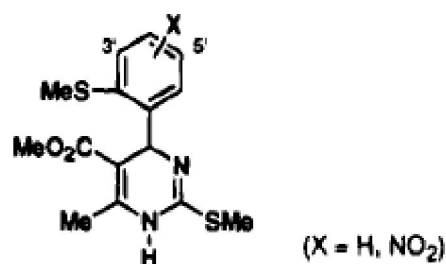


#### 4. Conclusion

Keeping in view the biological potential of Quinazoline derivatives, a methodology has been developed to synthesize new derivatives of Quinazolines viz. Quinazoline-2-thiols. For this, 2-[isothiocyanato(substituted phenyl)methyl]-3,4-dihydronaphthalene-1(2H)-ones were treated with primary aromatic amines. Also, Gaussian-03 studies of the prepared compounds have been carried out.

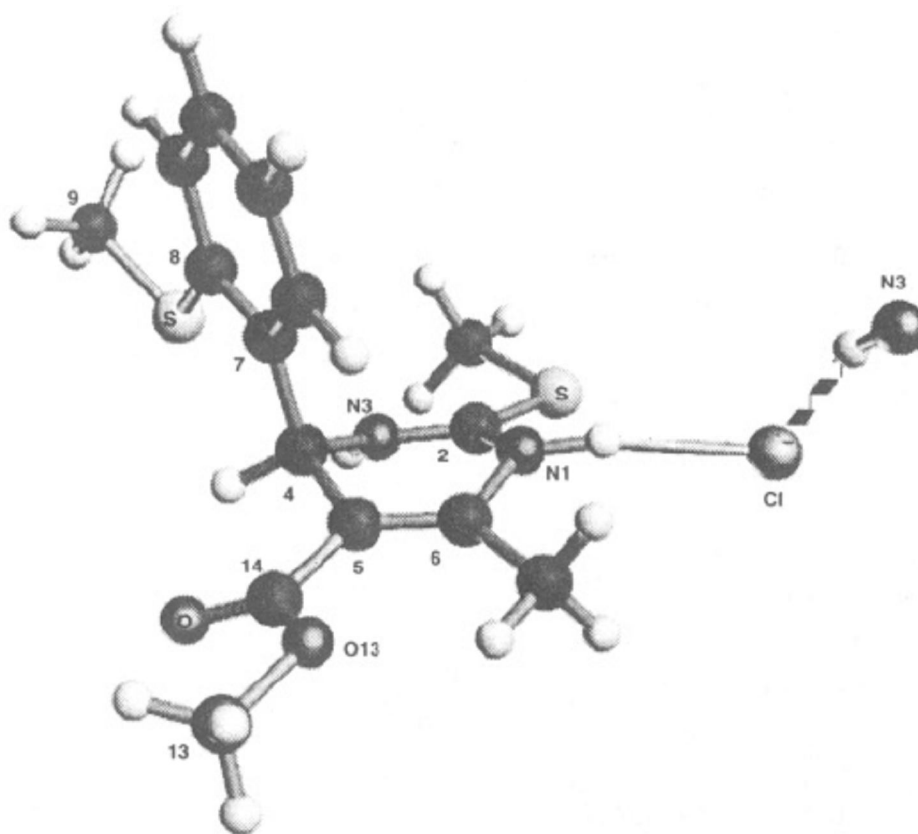
#### Computational Studies

As shown by the Gaussian 03 studies through the instrument, the stereochemistry of the synthesized compounds seems to be like the reported compounds (I) in the literature [9-13].



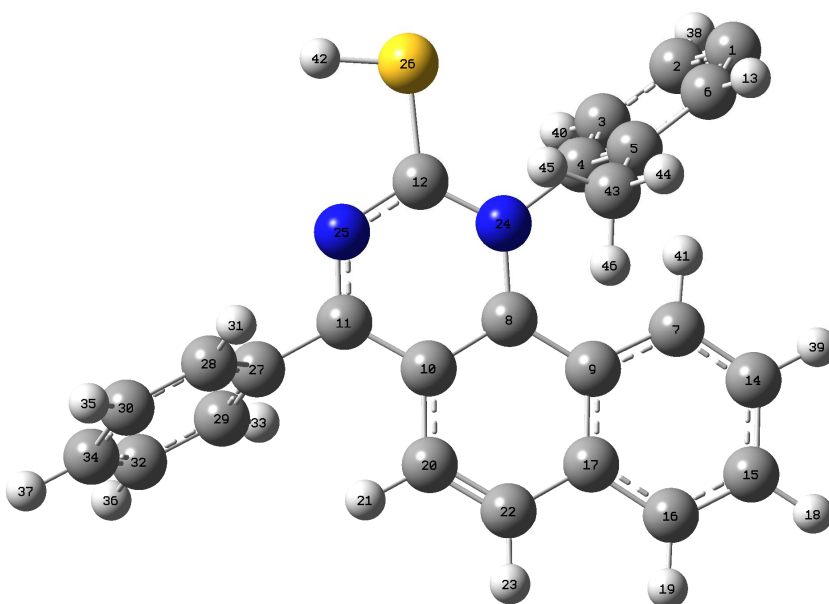
I

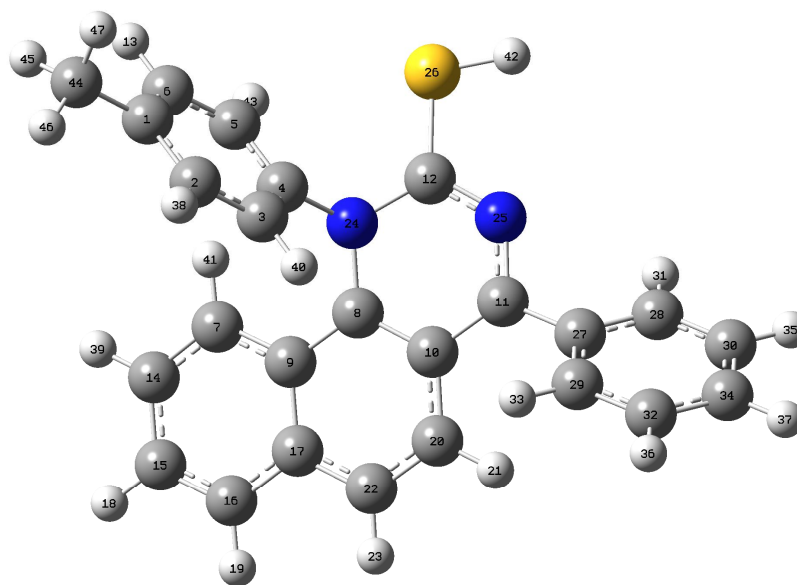




**Solid-state conformation of I as hydrochloride salt. Hydrogen bond distances: N1 – Cl = 3.088 Å<sup>0</sup>, N3 – Cl = 3.075 Å<sup>0</sup>**

The stereochemistry of the prepared compounds is given below showing that phenyl ring is not in the same plane as the rest of the molecule:





### Competing Interests

The authors declare that they have no competing interests.

### Authors' Contributions

All authors contributed more or less equally to this work.

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