
Kodihalli C. Ravindra, a Hosadu M. Vagdevi, b* and Vijayvithal P. Vaidya a

aDepartment of Chemistry, Kuvempu University, Jnana Sahyadri, Shankaraghatta-577451, Karnataka, India
bDepartment of Industrial Chemistry, Kuvempu University, Jnana Sahyadri, Shankaraghatta-577451, Karnataka, India
E-mail: vagdevihm@gmail.com

Abstract
Ethyl 3-aminonaphtho[2,1-b]furan-2-carboxylate 1 was converted into 3-amino-2-mercaptonaphthofuro[3,2-d]pyrimidin-4(3H)-one 4 by reacting it with carbon disulphide followed by methylation and condensation with hydrazine hydrate. The compound 4 on treatment with aryl isothiocyanates produced 2-arylaminoanilinonaphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-a]pyrimidin-5-ones 5(a-h). The title compounds 6(a-h) were obtained also by reacting 4 with aromatic acids in presence of phosphorus oxychloride. The structures of the newly synthesized compounds were confirmed by IR, 1H NMR, 13C NMR and mass spectral studies and elemental analysis. All the synthesized compounds have been screened for antimicrobial activity.

Keywords: Naphtho[2,1-b]furan, naphthofuropyrimidines, thiadiazolopyrimidines, phenyl isothiocyanates antimicrobial activity

Introduction
In the family of heterocyclic compounds, nitrogen-containing heterocycles with a sulfur atom are an important class of compounds in medicinal chemistry. There has been considerable interest in the development of preparative methods for the production of pyrimidines. This seems to be because pyrimidines represent one of the most active classes of compounds, possessing a wide spectrum of biological activity1-3. Pyrimidines and their ring-fused derivatives have a broad spectrum of biological activity; best known as the heterocyclic core of the nucleic acid bases. These ring systems are often incorporated into drugs designed for anticancer4,5, antiviral6, antihypertensive7, analgesic8, antipyretic9, antiinflammery10, antipsoriasis11 agents. Some of them are active on the blood circulatory system12 and can stimulate the skin preparative
regeneration and increase the efficacy of antibiotic therapy of *Staphylococcus* and *Proteus* infected wounds\(^\text{13}\). Similarly, derivatives of naphthofurans have attracted the attention of many organic chemists owing to their well pronounced activities such as anticancer\(^\text{14}\), antifungal and cytotoxic\(^\text{15}\) and in the treatment of metabolic disorders\(^\text{16}\). Hence, keeping these reports in view and continuation of our search for more potent naphthofuran derivatives\(^\text{17-20}\), we report in this paper the synthesis of novel condensed heterocyclic compounds encompassing bioactive molecules, i.e., pyrimidine, naphthofuran and also thiadiazole.

\[ \begin{align*}
\text{Scheme 1. General synthetic pathways for the preparation of naphtho[2,1-} & \text{b]furo-5H-[3,2-} \\
& \text{d][1,3,4]thiadiazolo[3,2-a]pyrimidin-5-ones.}\end{align*} \]
Results and Discussion

Amongst various methods used for construction of pyridinine\textsuperscript{21-24} ring the synthetic strategy involving o-amino ester as starting material\textsuperscript{25} was adopted in the present investigation. Thus treatment of ethyl 3-aminonaphtho[2,1-b]furan-2-carboxylate\textsuperscript{26} 1 with carbon disulphide and aqueous sodium hydroxide in dimethyl sulphoxide yielded a dithiocarbamate, ethyl 1-{[(sodiumthio)carbonothioyl]amino} naphtho[2,1-b]furan-2-carboxylate 2 as a salt, which (without isolating) was then methylated with dimethyl sulphate to afford a dithiocarbamate methyl ester, ethyl 1-{[(methylthio)carbonothioyl]amino}naphtho[2,1-b]furan-2-carboxylate 3. The structure of 3 was confirmed by IR, $^1$H NMR and mass spectral studies. The IR spectrum of 3 exhibited an absorption band at 1710 cm\textsuperscript{-1} due to the -C=O for an ester carbonyl group and 3055 cm\textsuperscript{-1} due to the -NH group. In the $^1$H NMR spectrum, a triplet at $\delta$ 1.4 due to three protons of the –CH\textsubscript{3} of an ester, a singlet at $\delta$ 2.35 integrating for the three protons of -SCH\textsubscript{3}, a quartet at $\delta$ 4.4 integrating for the two protons of –CH\textsubscript{2} of ester, multiplet at $\delta$ 7.4-8.2 for six aromatic protons and a broad singlet at $\delta$ 9.2 integrating for -NH (D\textsubscript{2}O exchangeable) proton were observed. The structure of 3 was further confirmed by mass spectral analysis. It exhibited a molecular ion peak at m/z 346 corresponding to its molecular weight. Compound 3 on reaction with hydrazine hydrate yielded the desired 3-amino-2-mercaptonaphthofuro[3,2-d]pyrimidin-4(3$H$)-one 4 in excellent yield. The IR spectrum of 4 exhibited an absorption band at 1673 cm\textsuperscript{-1} due to the -C=O and 3118 cm\textsuperscript{-1} due to the -NH\textsubscript{2} group. In the $^1$H NMR spectrum, a singlet at $\delta$ 2.8 due to the –SH proton, another broad singlet at $\delta$ 5.8 due to -NH\textsubscript{2} (D\textsubscript{2}O exchangeable) protons and a multiplet at $\delta$ 7.5-8.5 for six aromatic protons. The $^{13}$C NMR spectrum showed peaks at $\delta$ 169.39, 154.66 due to the -C=O and 133.29, 130.25, 129.79, 129.43, 128.93, 128.44, 127.89, 127.51, 125.25, 124.80, 123.93 and 122.40 were attributed to the twelve aromatic ring carbon atoms. Final proof for the structure was obtained by recording its mass spectrum, which exhibited a molecular ion peak at m/z 282, corresponding to its molecular weight.

Several synthetic routes are available for ring closure to obtain thiazolopyridines\textsuperscript{27-31}. One of the methods involves the reaction of compounds possessing o-aminothiazol functionality as in the case of compound 4, with aryl isothiocyanates. Thus compound 4 on reaction with various aryl isothiocyanates yielded 2-arylaminonaphthofuro[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-a]pyrimidin-5-ones 5(a-h). The structure of the compound 5a was elucidated from spectroscopic data. The IR spectrum of 5a exhibited an absorption band at 1676 cm\textsuperscript{-1} due to the -C=O group and at 3059 cm\textsuperscript{-1} due to –NH group. The $^1$H NMR spectrum of 5a exhibited a multiplet at $\delta$ 7.54-8.55 for ten aromatic protons and a broad singlet at $\delta$ 9.38 due to -NH (D\textsubscript{2}O exchangeable) proton. The molecular ion peak at m/z 384 in its mass spectrum confirmed the structure 5a.

The compounds having o-aminomercapto functionality are also known to undergo cyclization on treatment with aromatic acids in presence of phosphorus oxychloride. Thus reaction of 4, having similar functionality, on treatment with different aromatic acids in
phosphorus oxychloride led to the formation of 2-aryl naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-a]pyrimidin-5-ones 6(a-d). The IR spectrum of 6a exhibited an absorption band at 1663 cm⁻¹ due to the -C=O group. In the ¹H NMR spectrum, only a multiplet at δ 7.5-8.1 for eleven aromatic protons was observed. The structure of 6a was further confirmed by mass spectral analysis. It exhibited a molecular ion peak at m/z 369 corresponding to its molecular weight. Similarly all the compounds were purified by column chromatography and characterized by spectroscopic studies. The reaction pathway is depicted in Scheme 1.

**Evaluation of antimicrobial activity**
The *in vitro* antimicrobial activity was carried out by cup-plate method. All the synthesized compounds were screened for antibacterial activity against *Escherichia coli*, *Micrococcus luteus* and *Staphylococcus aureus* using Chloramphenicol (0.001 mole/ml) as standard. The antifungal activity was investigated against *Aspergillus flavus*, *Aspergillus niger* and *Curvulriaria lunata* using Flucanazole (0.001 mole/ml) as standard. Inhibition was recorded by measuring the diameter of the inhibition zone at the end of 24 hr for bacteria and 48 hr for fungi. Each experiment was repeated thrice and the average of the three independent determinations was recorded. The results are summarized in Table 1.

**Table 1. Antimicrobial activity of the compounds**

<table>
<thead>
<tr>
<th>Compound</th>
<th>Antibacterial activity Zone of Inhibition in mm</th>
<th>Antifungal activity Zone of Inhibition in mm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[<em>E.coli</em>] [<em>M.luteus</em>] [<em>S.aureus</em>]</td>
<td>[<em>A.flaves</em>] [<em>A.niger</em>] [<em>C.lunata</em>]</td>
</tr>
<tr>
<td>3</td>
<td>18    11 10</td>
<td>13 10 12</td>
</tr>
<tr>
<td>4</td>
<td>33    35 23</td>
<td>12 15 15</td>
</tr>
<tr>
<td>5a</td>
<td>18    15 14</td>
<td>14 12 13</td>
</tr>
<tr>
<td>5b</td>
<td>29    27 26</td>
<td>15 14 12</td>
</tr>
<tr>
<td>5c</td>
<td>28    27 15</td>
<td>22 21 22</td>
</tr>
<tr>
<td>5d</td>
<td>23    19 12</td>
<td>12 10 10</td>
</tr>
<tr>
<td>5e</td>
<td>17    19 20</td>
<td>11 10 12</td>
</tr>
<tr>
<td>5f</td>
<td>22    20 22</td>
<td>11 12 11</td>
</tr>
<tr>
<td>5g</td>
<td>32    29 21</td>
<td>13 14 08</td>
</tr>
<tr>
<td>5h</td>
<td>20    33 21</td>
<td>16 17 23</td>
</tr>
<tr>
<td>6a</td>
<td>20    26 25</td>
<td>17 12 15</td>
</tr>
<tr>
<td>6b</td>
<td>33    36 34</td>
<td>11 12 15</td>
</tr>
<tr>
<td>6c</td>
<td>18    26 22</td>
<td>12 16 13</td>
</tr>
<tr>
<td>6d</td>
<td>17    20 19</td>
<td>15 09 11</td>
</tr>
<tr>
<td>Standard</td>
<td>38    37 44</td>
<td>16 19 16</td>
</tr>
<tr>
<td>DMF</td>
<td>+ ve</td>
<td>+ ve</td>
</tr>
</tbody>
</table>

+ve indicates growth of microbes. Control: DMF (0.01% solution in distilled water). Standard for antibacterial: Chloramphenicol (0.001 mole/ml). Standard for antifungal: Flucanazole (0.001 mole/ml).
Amongst the compounds tested for antibacterial activity, the compound 6b was found to display considerable activity against all the bacteria, whereas compound 4 was found to exhibit promising activity against E. coli and M. luteus. The compound 5c showed more antifungal activity than the standard flucanazole and the compound 5h exhibited almost equipotent activity against A. flaves and A. niger and was found to be more active than the standard against C. lunata.

**Experimental Section**

**General Procedures.** Melting points were determined in open capillary tubes and are uncorrected. IR spectra were recorded in KBr on FT-IR (Research Spectrophotometer Series) and Perkin-Elmer FT-IR (Spectrum 1000); $^1$H NMR and $^{13}$C NMR spectra on a Bruker AMX (400 MHz) Spectrophotometer using DMSO-$d_6$ as solvent and TMS as an internal standard (chemical shifts in $\delta$) and mass spectra on a LC-MS instrument. Compounds were checked for their purity by TLC on silica gel G plates and spots were located by iodine vapors. Satisfactory C, H, N analyses were obtained for all the compounds.

**Ethyl 1-{[(methylthio)carbonothioyl]amino}naphtho[2,1-b]furan-2-carboxylate (3).** To a vigorously stirred solution of ethyl 3-aminonaphtho[2,1-b]furan-2-carboxylate 1 (4.18 g, 0.02 mole) in dimethyl sulphoxide (10 ml) at room temperature, carbon disulphide (1.6 ml, 0.26 mole) and aqueous sodium hydroxide (1.2 ml, 2 M) were added drop wise. After 30 min, dimethyl sulphate (2.5 g, 0.025 mole) was added under cooling in an ice bath. Stirring was continued for 1 hr and then the reaction mixture was poured in ice water. The solid that separated out was filtered, dried and recrystalized from ethanol. (5.26 g, 93 %), Mp. 195-197°C, MS: (M+) 345; Anal. Calcd for C$_{17}$H$_{15}$NO$_3$S$_2$: C, 59.02; H, 4.29; N, 4.01; Found: C, 58.65; H, 4.12; N, 4.00.

**3-Amino-2-mercaptonaphtho[2,1-b]furo[3,2-d]pyrimidin-4(3H)-one (4).** A solution of ethyl-1-{[(methylthio)carbonothioyl]aminonaphtho[2,1-b]furan-2-carboxylate 3 (2.89 g, 0.01 mole) in ethanol (30 ml) was treated with hydrazine hydrate (5.0 g, 0.1 mole) and refluxed on water bath for 8 hr. After cooling, the solid obtained was filtered, dried and recrystallized from 1:1 ethyl acetate and hexane. (2.02g, 85 %), Mp. 212-214°C, MS: (M$^+$) 283; Anal. Calcd for C$_{14}$H$_9$N$_3$O$_2$S: C, 59.35; H, 3.20; N, 14.83. Found: C, 59.53; H, 3.11; N, 14.42.


A mixture of 3-amino-2-mercaptonaphthofuro[3,2-d]pyrimidin-4(3H)-one 4, a pinch of potassium carbonate (anhyd) and appropriate phenyl isothiocyanates in DMF (20 ml) was refluxed in an oil bath maintained at 150°C for 36 hr. The reaction mixture was poured into ice-cold water, the solid that separated out was filtered, dried and recrystallized from ethanol to yield 5 (a-h).
2-Anilinonaphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiazolo[3,2-a]pyrimidin-5-one (5a). Yellow amorphous, compound 4 (250 mg, 0.8 m mole), phenyl isothiocyanate (0.105 ml, 0.7 m mole), (305 mg, 90 %), Mp. 245-247 °C. IR (KBr, cm⁻¹): 1619 (C=N), 1672 (C=O). ¹H NMR (400 MHz, DMSO): δ 7.54-8.55 (m, 11H, Ar), 9.38 (brs, 1H, NH), ¹³C NMR (DMSO) δ: 112.35, 114.13, 122.07, 124.87, 127.73, 128.63, 128.82, 129.60, 130.32, 131.28, 132.33, 134.92, 136.26, 137.52, 139.66, 140.78, 141.12, 144.81, 153.06, 154.64, 167.24. MS: (M⁺) m/z 384. Anal. Calcd for C₂₁H₁₂N₄O₂S (384): C, 65.61; H, 3.15; N, 14.57. Found: C, 65.53; H, 3.11; N, 14.45.

2-[(3-Chlorophenyl)amino]naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiazolo[3,2-a]pyrimidin-5-one (5b). Yellow solid, compound 4 (250 mg, 0.8 m mole), 3-chlorophenyl isothiocyanate (135 mg, 0.8 m mole), (284 mg, 77 %), Mp. 237-239 °C, IR (KBr, cm⁻¹): 1621 (C=N), 1668 (C=O). ¹H NMR (400 MHz, DMSO): δ 7.24-8.35 (m, 10H, Ar), 9.45 (brs, 1H, NH), ¹³C NMR (DMSO) δ: 113.26, 114.12, 122.10, 122.79, 124.84, 125.64, 127.72, 128.63, 128.83, 129.63, 130.33, 131.25, 134.54, 136.26, 137.54, 137.83, 141.09, 144.82, 146.45, 153.05, 166.44. MS: (M⁺) m/z, 419. Anal. Calcd for C₂₁H₁₁N₄O₂SCl (419): C, 60.22; H, 2.65; N, 13.38. Found: C, 60.15; H, 2.51; N, 13.27.

2-[(4-Chlorophenyl)amino]naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiazolo[3,2-a]pyrimidin-5-one (5c). Brown solid, compound 4 (250 mg, 0.8 m mole), 4-chlorophenyl isothiocyanate (135 mg, 0.8 m mole), (269 mg, 73 %), Mp. 265-267 °C, IR (KBr, cm⁻¹): 1618 (C=N), 1659 (C=O). ¹H NMR (400 MHz, DMSO): δ 7.16-8.28 (m, 10H, Ar), 9.68 (brs, 1H, NH), ¹³C NMR (DMSO) δ: 113.78, 114.15, 116.72, 122.09, 123.12, 124.85, 127.71, 127.94, 128.64, 128.84, 129.63, 130.31, 131.25, 136.28, 137.53, 141.09, 142.87, 144.83, 147.01, 153.06, 166.57. MS: (M⁺), m/z, 419; Anal. Calcd for C₂₁H₁₁N₄O₂SCl (419): C, 60.22; H, 2.65; N, 13.38. Found: C, 60.15; H, 2.51; N, 13.27.

2-[(3-Methoxyphenyl)amino]naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiazolo[3,2-a]pyrimidin-5-one (5d). Brown solid, compound 4 (250 mg, 0.8 m mole), 3-methoxyphenyl isothiocyanate (0.132 ml, 0.8 m mole), (299 mg, 82 %), Mp. 241-243 °C, IR (KBr, cm⁻¹): 1627 (C=N), 1666 (C=O). ¹H NMR (400 MHz, DMSO): δ 3.89 (s, 3H, OCH₃), 7.25-8.16 (m, 10H, Ar), 9.27 (brs, 1H, NH), ¹³C NMR (DMSO) δ: 56.38, 112.48, 113.19, 116.82, 122.39, 124.12, 124.91, 126.77, 127.84, 128.53, 129.14, 129.73, 130.52, 131.16, 137.18, 137.63, 141.39, 141.90, 144.72, 147.61, 152.17, 169.35. MS: (M⁺), m/z, 414; Anal. Calcd for C₂₂H₁₄N₄O₃S (414): C, 63.76; H, 3.40; N, 13.52; Found: C, 63.64; H, 3.37; N, 13.45.

2-[(4-Methoxyphenyl)amino]naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiazolo[3,2-a]pyrimidin-5-one (5e). Brown solid, compound 4 (250 mg, 0.8 m mole), 4-methoxyphenyl isothiocyanate (0.132 ml, 0.8 m mole), (235 mg, 89 %), Mp. 238-240 °C, IR (KBr, cm⁻¹): 1631 (C=N), 1668 (C=O). ¹H NMR (400 MHz, DMSO): δ 3.92 (s, 3H, OCH₃), 7.15-8.35 (m, 10H, Ar), 9.33 (brs, 1H, NH), ¹³C NMR (DMSO) δ: 58.56, 110.26, 113.17, 121.19, 122.85, 124.44, 125.76, 126.47, 128.81, 128.97, 129.77, 130.57, 131.13, 134.73, 136.21, 137.14, 138.63, 142.19, 144.43, 145.47, 152.55, 168.26. MS: (M⁺), m/z, 414; Anal. Calcd for C₂₂H₁₄N₄O₃S (414): C, 63.76; H, 3.40; N, 13.52. Found: C, 63.68; H, 3.32; N, 13.43.
2-[(4-Methylphenyl)amino]naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-a]pyrimidin-5-one (5f). Brown solid, compound 4 (250 mg, 0.8 m mole), 4-methylphenyl isothiocyanate (0.119 ml, 0.8 m mole), (260 mg, 74 %), Mp. 231-233 0C, IR (KBr, cm\(^{-1}\)): 1629 (C=N), 1671 (C=O). \(^1\)H NMR (400 MHz, DMSO): \(\delta\) 2.1 (s, 3H, CH₃), 7.20-8.15 (m, 11H, Ar), 9.10 (brs, 1H, NH), 13 C NMR (DMSO) \(\delta\): 35.45, 112.71, 114.52, 115.67, 121.69, 123.12, 124.85, 126.83, 127.97, 128.64, 129.64, 130.63, 133.36, 134.27, 136.29, 138.31, 142.49, 143.61, 144.63, 146.59, 154.46, 162.31. MS: (M\(^{+}\)) m/z, 398; Anal. Calcd for C\(_{22}\)H\(_{14}\)N\(_4\)O\(_2\)S (398): C, 66.32; H, 3.54; N, 14.06. Found: C, 66.24; H, 3.23; N, 14.01.

2-[(3-Nitrophenyl)amino]naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-a]pyrimidin-5-one (5g). Yellow solid, compound 4 (250 mg, 0.8 m mole), 3-nitrophenyl isothiocyanate (159 mg, 0.88 m mole), (280 mg, 69 %), Mp. 267-269 0C, IR (KBr, cm\(^{-1}\)): 1635 (C=N), 1677 (C=O). \(^1\)H NMR (400 MHz, DMSO): \(\delta\) 7.54-8.41 (m, 11H, Ar), 9.65 (brs, 1H, NH), 13 C NMR (DMSO) \(\delta\): 111.37, 114.36, 122.42, 122.95, 123.68, 125.53, 126.89, 128.76, 128.91, 129.58, 130.25, 132.42, 134.54, 136.69, 137.83, 138.59, 142.36, 143.69, 145.31, 154.79, 163.34. MS: (M\(^{+}\)), m/z, 429; Anal. Calcd for C\(_{21}\)H\(_{11}\)N\(_5\)O\(_4\)S (429): C, 58.74; H, 2.58; N, 16.31. Found: C, 58.70; H, 2.31; N, 16.19.

2-[(4-Nitrophenyl)amino]naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-a]pyrimidin-5-one (5h). Yellow solid, compound 4 (250 mg, 0.8 m mole), 4-nitrophenyl isothiocyanate (159 mg, 0.88 m mole), (261 mg, 86 %), Mp. 255-257 0C, IR (KBr, cm\(^{-1}\)): 1623 (C=N), 1686 (C=O). \(^1\)H NMR (400 MHz, DMSO): \(\delta\) 7.48-8.39 (m, 11H, Ar), 9.64 (brs, 1H, NH), 13 C NMR (DMSO) \(\delta\): 112.21, 113.66, 122.53, 122.86, 123.37, 125.98, 126.65, 128.36, 128.41, 130.29, 133.23, 134.75, 136.39, 137.52, 138.19, 142.56, 143.72, 145.35, 153.97, 164.42. MS: (M\(^{+}\)), m/z, 429; Anal. Calcd for C\(_{21}\)H\(_{11}\)N\(_5\)O\(_4\)S (429): C, 58.74; H, 2.58; N, 16.31; Found: C, 58.63; H, 2.34; N, 16.25.

A mixture of 4 (0.001 mole) and different appropriate aromatic acids (0.001 mole) in phosphorous oxychloride (10 ml) was heated on an oil bath at 120 0C for 1 hr. The reaction mixture was cooled, poured into ice and neutralized with aqueous potassium carbonate solution. The solid thus separated was filtered, washed thoroughly with water and recrystallised from ethanol to yield 6 (a-d).
2-(4-Nitrophenyl)naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-]pyrimidin-5-one (6b). Yellow solid, compound 4 (300 mg, 0.001 mole), 4-nitrobenzoic acid (167 mg, 0.001 mole), (364 mg, 83 %), Mp. 233-235 °C, IR (KBr, cm⁻¹): 1622 (C=N), 1669 (C=O). ¹H NMR (400 MHz, DMSO): δ 7.16-8.25 (m, 10H, Ar), ¹³C NMR (DMSO) δ: 112.34, 114.59, 116.32, 121.33, 122.16, 124.43, 126.47, 127.84, 128.53, 129.14, 130.73, 131.52, 135.36, 137.28, 138.62, 142.39, 144.59, 145.62, 147.68, 153.57, 163.34. MS: (M⁺), m/z, 414; Anal. Calcd for C₂₁H₁₀N₄O₄S (414): C, 60.87; H, 2.43; N, 13.52. Found: C, 60.82; H, 2.34; N, 13.43.

2-(4-Chlorophenyl)naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-]pyrimidin-5-one (6c). Brown solid, compound 4 (300 mg, 0.001 mole), 3-chloro benzoic acid (156 mg, 0.001 mole), (376 mg, 88 %), Mp. 227-229 °C, IR (KBr, cm⁻¹): 1618 (C=N), 1659 (C=O). ¹H NMR (400 MHz, DMSO): δ 7.31-8.25 (m, 10H, Ar), ¹³C NMR (DMSO) δ: 111.68, 114.17, 121.79, 122.97, 124.42, 125.56, 126.45, 128.62, 128.96, 129.64, 130.51, 131.41, 134.32, 136.24, 137.52, 138.64, 142.19, 144.43, 146.48, 153.95, 165.32. MS: (M⁺), m/z, 404; Anal. Calcd for C₂₁H₁₀N₃O₂SCl (404): C, 62.46; H, 2.50; N, 10.41. Found: C, 62.39; H, 2.46; N, 10.32.

2-(4-Aminophenyl)naphtho[2,1-b]furo-5H-[3,2-d][1,3,4]thiadiazolo[3,2-]pyrimidin-5-one (6d). Brown solid, compound 4 (300 mg, 0.001 mole), 4-amino benzoic acid (137 mg, 0.001 mole), (317 mg, 78 %), Mp. 213-215 °C, IR (KBr, cm⁻¹): 1629 (C=N), 1672 (C=O). ¹H NMR (400 MHz, DMSO): δ 5.24 (brs, 2H, NH₂), 7.18-8.26 (m, 10H, Ar), ¹³C NMR (DMSO) δ: 113.52, 114.72, 118.61, 122.63, 123.42, 124.45, 126.83, 127.68, 128.64, 129.47, 130.49, 132.76, 134.29, 136.53, 138.31, 142.49, 143.25, 144.63, 146.36, 154.61, 167.34. MS: (M⁺), m/z, 384; Anal. Calcd for C₂₁H₁₂N₄O₂S (384): C, 65.61; H, 3.15; N, 14.57. Found: C, 65.51; H, 3.08; N, 14.51.

Acknowledgements

The authors are thankful to Professor and Chairman, Department of Studies and Research in Chemistry, Kuvempu University for providing laboratory facilities. Authors are also thankful to the Head, RSIC, Indian Institute of Science, Bangalore for spectral data.

References