



## A competent multi component synthesis new triazolopyrimidines

<sup>a</sup>Piyush D. Fadadu, <sup>a</sup>Purvisha P. Fadadu, <sup>b</sup>Kiran S. Nimavat, <sup>c</sup>Kartik B. Vyas\*

<sup>a</sup>JJT University, Jhunjhunu, Rajasthan

<sup>b</sup>Government Science college, Gandhinagar

<sup>c</sup>Sheth L.H. Science College, Mansa.

---

### ABSTRACT

A series of novel derivatives of triazolopyrimidines were synthesized by a one-pot reaction of 3-amino-1,2,4-triazole, different acetoacetamides and aryl aldehydes in using heating within 30 min. The structures of the target compounds were confirmed by inspection of their <sup>1</sup>H-NMR, IR and MS spectra. The advantages of this method are short reaction times, good yields, high selectivity and operational simplicity.

**Keywords:** [1,2,4]triazolo[1,5-a]pyrimidines, acetoacetamides, triazole condensation synthesis.

---

### INTRODUCTION

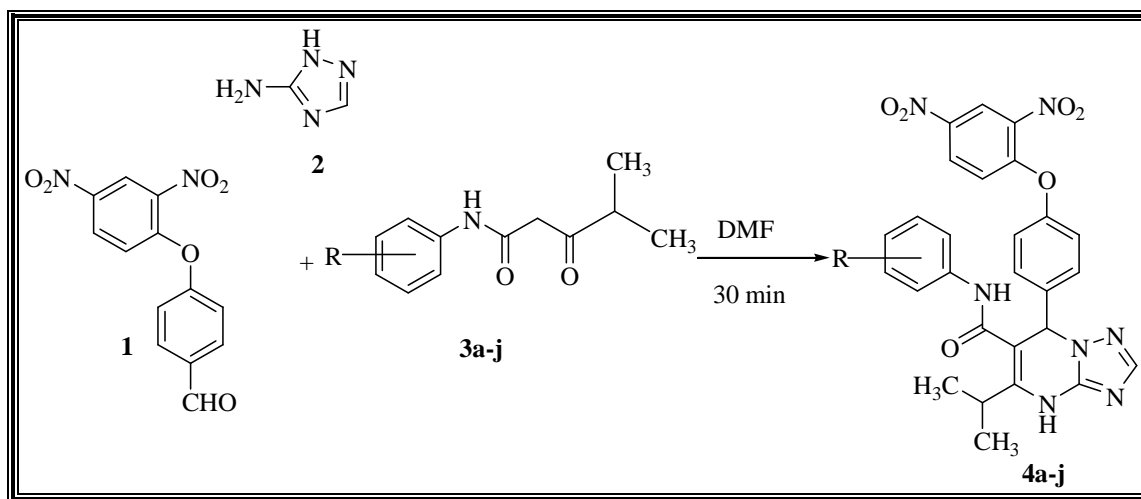
The condensation of a ring of 1,2,4-triazole and another one of pyrimidine gives rise to the formation of bicyclic heterocycles known as 1,2,4-triazolopyrimidines. Four different possibilities exist for the relative orientation of both rings, so four different isomeric families of compounds are defined (see Fig. 1). Among these, 1,2,4-triazolo[1,5-a]pyrimidine derivatives are thermodynamically more stable and, thus, the most studied ones<sup>[1]</sup>, a few of them being commercially available. Revisions surveying the synthesis, reactivity, spectroscopic characterization and crystallographic studies of 1,2,4-triazolo[1,5-c]pyrimidines<sup>[2]</sup> 1,2,4-triazolo[4,3-a]pyrimidines<sup>[3]</sup> and 1,2,4-triazolo[4,3-c]pyrimidines<sup>[4]</sup> have also been published.

The studies about the coordination chemistry of triazolopyrimidines have been exclusively focused till now in the 1,5-a series. These compounds, which are structurally similar and may be regarded as mimic of isomeric purines, have displayed a rich coordination chemistry, a considerable number of new compounds with interesting structural features having been characterized<sup>[5]</sup>, including simple mononuclear compounds with monodentately coordinated ligands<sup>[6,7]</sup> and di or polynuclear compounds in which either the triazolopyrimidine ligand<sup>[8]</sup> or other auxiliary ligands<sup>[9]</sup> bridge the metalatoms.

From the standpoint of biological activity, fused heteroaromatic systems are often of much greater interest than the constituent monocyclic compounds. Recently, 1,2,4-triazolo[1,5-a]pyrimidines have aroused increasing attention from the chemical and biological view points, due to their diverse pharmacological activities, such as antitumor potency, inhibition of KDR kinase, antifungal effect and macrophage activation. They have proved to be promising anticancer agents with dual mechanisms of tubulin polymerization promotion as well as cyclin dependent kinases 2 inhibition. Some examples of published derivatives of 1,2,4-triazolo[1,5-a]pyrimidine with their biological activities.

Several synthetic strategies have been reported for the preparation of triazolopyrimidine derivatives.<sup>[10, 11-15]</sup> Most of these are based on modification of the classical one-pot Biginelli reaction<sup>[10, 11-14]</sup> and in some cases on more complex multi-step processes involving harsh reaction conditions and long reaction times.<sup>[16-17]</sup> One major drawback of the classical Biginelli protocol is the low yield that is frequently encountered when using sterically more demanding aldehydes.

To circumvent these problems, we have developed a new microwave assisted protocol for the synthesis of novel pyrimidines (**4a-j**) with the advantage of short reaction time, high yield and environmentally friendliness (**Scheme-a**).



Scheme-a

## EXPERIMENTAL SECTION

Melting points were measured in open capillaries and are uncorrected. <sup>1</sup>HNMR spectra were recorded on Bruker spectrophotometer (400MHz). Chemical shifts are expressed in units relative to TMS signal as internal reference. IR spectra were recorded on FT-IR Shimadzu-FT-IR 8400 spectrophotometer on KBr pallets. Mass spectra were recorded on GCMS QP2010 Gas Chromatograph. Thin Layer Chromatography was performed on silica gel-G using hexane: ethylacetate solvent system.

### Typical experimental procedure for the synthesis of triazolopyrimidines.

A mixture of the 3-amino-1,2,4-triazole (2 mmol), a suitable acetoacetamide (1 mmol) and 4-(2,4-dinitrophenoxy)benzaldehyde (1 mmol) was refluxed in 0.5 ml of DMF for 30 min. After cooling, methanol (~15 ml) was added. The reaction mixture was allowed to stand overnight and then filtered to give the solid triazolopyrimidine products, which were crystallized from ethanol.

### 7-(4-(2,4-dinitrophenoxy)phenyl)-N-(3-chlorophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-

**a]**pyrimidine-6-carboxamide **4a**. m.p. 194°C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.13) (s, 3H, H<sub>a</sub>), (δ 1.19) (s, 3H, H<sub>b</sub>), (δ 2.42) (d, 1H, H<sub>c</sub>), (δ 6.46) (s, 1H, H<sub>d</sub>), (δ 6.70-6.72) (d, 2H, H<sub>e,e'</sub>), (δ 6.80-6.83) (d, 1H, H<sub>f</sub>), (δ 7.02-7.06) (t, 2H, H<sub>g,g'</sub>), (δ 7.12-7.18) (t, 1H, H<sub>h</sub>), (δ 7.20-7.28) (m, 3H, H<sub>i,k</sub>), (δ 7.34-7.38) (dd, 2H, H<sub>m</sub>), (δ 7.58) (s, 1H, H<sub>n</sub>), (δ 9.87) (s, 1H, H<sub>o</sub>), (δ 10.05) (s, 1H, H<sub>p</sub>). FT IR (cm<sup>-1</sup>): 3245 (N-H stretching of secondary amine), 3024 (C-H stretching of aromatic ring), 2915 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2856 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1654 (C=O stretching of amide), 1600 (C=N stretching of triazole ring), 1557 (N-H deformation of pyrimidine ring), 1508 and 1476 (C=C stretching of aromatic ring), 1485 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1402 (C-H symmetrical deformation of CH<sub>3</sub> group), 1321 (C-N stretching), 1257 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1238 (C-O-C stretching), 1034 (C-H in plane deformation of aromatic ring), 831 (C-H out of plane bending of 1,4-disubstitution), 728 (C-Cl stretching), Mass: *m/z* 576; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>ClN<sub>7</sub>O<sub>6</sub>: C, 54.99; H, 3.31; Cl, 6.47; N, 17.59; O, 17.52; Found: C, 54.15; H, 3.21; Cl, 6.14; N, 17.72; O, 17.03%.

**7-(4-(2,4-dinitrophenoxy) phenyl)-N-(4-fluorophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4b.** m.p. 198 °C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.11) (s, 3H, H<sub>a</sub>), (δ 1.15) (s, 3H, H<sub>b</sub>), (δ 2.38) (d, 1H, H<sub>c</sub>), (δ 6.34) (s, 1H, H<sub>d</sub>), (δ 6.67-6.76) (d, 2H, H<sub>ee'</sub>), (δ 6.82-6.89) (d, 1H, H<sub>f</sub>), (δ 7.03-7.09) (t, 2H, H<sub>gg'</sub>), (δ 7.17-7.37) (dd'dd', 4H, H<sub>hh'-ii'</sub>), (δ 7.49-7.54) (dd, 2H, H<sub>jk</sub>), (δ 7.63) (s, 1H, H<sub>l</sub>), (δ 9.67) (s, 1H, H<sub>m</sub>), (δ 10.13) (s, 1H, H<sub>n</sub>). FT IR (cm<sup>-1</sup>): 3243 (N-H stretching of secondary amine), 3013 (C-H stretching of aromatic ring), 2942 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2845 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1657 (C=O stretching of amide), 1608 (C=N stretching of triazole ring), 1545 (N-H deformation of pyrimidine ring), 1512 and 1474 (C=C stretching of aromatic ring), 1450 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1408 (C-H symmetrical deformation of CH<sub>3</sub> group), 1325 (C-N stretching), 1270 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1247 (C-O-C stretching), 1025 (C-H in plane deformation of aromatic ring), 828 (C-H out of plane bending of 1,4-disubstitution), 730 (C-Cl stretching), Mass: *m/z* 559; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>FN<sub>7</sub>O<sub>6</sub>: C, 57.00; H, 3.25; F, 3.37; N, 18.45; O, 18.00; Found: C, 56.88; H, 3.21; F, 3.01; N, 18.40; O, 17.80%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(4-chlorophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4c.** m.p. 187 °C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.15) (s, 3H, H<sub>a</sub>), (δ 1.17) (s, 3H, H<sub>b</sub>), (δ 2.40) (d, 1H, H<sub>c</sub>), (δ 6.14) (s, 1H, H<sub>d</sub>), (δ 6.64-6.68) (d, 2H, H<sub>ee'</sub>), (δ 6.70-6.84) (d, 1H, H<sub>f</sub>), (δ 7.00-7.10) (t, 2H, H<sub>gg'</sub>), (δ 7.24-7.38) (dd'dd', 4H, H<sub>hh'-ii'</sub>), (δ 7.45-7.50) (dd, 2H, H<sub>jk</sub>), (δ 7.69) (s, 1H, H<sub>l</sub>), (δ 9.64) (s, 1H, m), (δ 10.05) (s, 1H, H<sub>n</sub>). FT IR (cm<sup>-1</sup>): 3159 (N-H stretching of secondary amine), 3024 (C-H stretching of aromatic ring), 2945 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2854 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1645 (C=O stretching of amide), 1601 (C=N stretching of triazole ring), 1554 (N-H deformation of pyrimidine ring), 1500 and 1435 (C=C stretching of aromatic ring), 1440 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1423 (C-H symmetrical deformation of CH<sub>3</sub> group), 1312 (C-N stretching), 1223 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1221 (C-O-C stretching), 1024 (C-H in plane deformation of aromatic ring), 823 (C-H out of plane bending of 1,4-disubstitution), 721 (C-Cl stretching), Mass: *m/z* 576; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>ClN<sub>7</sub>O<sub>6</sub>: C, 55.60; H, 3.51; Cl, 6.47; N, 17.89; O, 17.52; Found: C, 55.18; H, 3.13; Cl, 6.25; N, 17.71; O, 17.05%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(4-nitrophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4d.** m.p. 203 °C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.13) (s, 3H, H<sub>a</sub>), (δ 1.19) (s, 3H, H<sub>b</sub>), (δ 2.42) (d, 1H, H<sub>c</sub>), (δ 6.30) (s, 1H, H<sub>d</sub>), (δ 6.50-6.60) (d, 2H, H<sub>ee'</sub>), (δ 6.71-6.79) (d, 1H, H<sub>f</sub>), (δ 7.02-7.08) (t, 2H, H<sub>gg'</sub>), (δ 7.15-7.34) (dd'dd', 4H, H<sub>hh'-ii'</sub>), (δ 7.41-7.46) (dd, 2H, H<sub>kl</sub>), (δ 7.56) (s, 1H, H<sub>m</sub>), (δ 9.58) (s, 1H, H<sub>n</sub>), (δ 10.02) (s, 1H, H<sub>o</sub>). FT IR (cm<sup>-1</sup>): 3216 (N-H stretching of secondary amine), 3021 (C-H stretching of aromatic ring), 2951 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2851 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1635 (C=O stretching of amide), 1665 (C=N stretching of triazole ring), 1545 (N-H deformation of pyrimidine ring), 1504 and 1435 (C=C stretching of aromatic ring), 1411 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1402 (C-H symmetrical deformation of CH<sub>3</sub> group), 1312 (C-N stretching), 1224 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1229 (C-O-C stretching), 1028 (C-H in plane deformation of aromatic ring), 843 (C-H out of plane bending of 1,4-disubstitution), 738 (C-Cl stretching), Mass: *m/z* 576; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>N<sub>8</sub>O<sub>8</sub>: C, 54.47; H, 3.15; N, 20.06; O, 22.92; Found: C, 54.28; H, 3.02; N, 20.01; O, 22.76%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(3-nitrophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4e.** m.p. 189°C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.13) (s, 3H, H<sub>a</sub>), (δ 1.19) (s, 3H, H<sub>b</sub>), (δ 2.42) (d, 1H, H<sub>c</sub>), (δ 6.56) (s, 1H, H<sub>d</sub>), (δ 6.71-6.73) (d, 2H, H<sub>ee'</sub>), (δ 6.82-6.84) (d, 1H, H<sub>f</sub>), (δ 7.02-7.06) (t, 2H, H<sub>gg'</sub>), (δ 7.12-7.16) (t, 1H, H<sub>h</sub>), (δ 7.23-7.31) (m, 3H, H<sub>j-k</sub>), (δ 7.42-7.46) (dd, 2H, H<sub>lm</sub>), (δ 7.63) (s, 1H, H<sub>n</sub>), (δ 9.65) (s, 1H, H<sub>o</sub>), (δ 10.23) (s, 1H, H<sub>p</sub>). FT IR (cm<sup>-1</sup>): 3267 (N-H stretching of secondary amine), 3025 (C-H stretching of aromatic ring), 2912 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2845 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1665 (C=O stretching of amide), 1615 (C=N stretching of triazole ring), 1527 (N-H deformation of pyrimidine ring), 1516 and 1454 (C=C stretching of aromatic ring), 1413 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1411 (C-H symmetrical deformation of CH<sub>3</sub> group), 1363 (C-N stretching), 1251 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1215 (C-O-C stretching), 1039 (C-H in plane deformation of aromatic ring), 828 (C-H out of plane bending of 1,4-disubstitution), 731 (C-Cl stretching), Mass: *m/z* 576; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>N<sub>8</sub>O<sub>8</sub>: C, 53.97; H, 3.21; N, 20.09; O, 22.99; Found: C, 53.80; H, 3.33; N, 19.69; O, 22.62%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(4-hydroxyphenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4f.** m.p. 184 °C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.13) (s, 3H, H<sub>a</sub>), (δ 1.19) (s, 3H, H<sub>b</sub>), (δ 2.42) (d, 1H, H<sub>c</sub>), (δ 6.52) (s, 1H, H<sub>d</sub>), (δ 6.48-6.58) (d, 2H, H<sub>ee'</sub>), (δ 6.64-6.74) (d, 1H, H<sub>f</sub>), (δ 7.05-7.11) (t, 2H, H<sub>gg'</sub>), (δ 7.16-7.29) (dd'dd', 4H, H<sub>hh'-ii'</sub>), (δ 7.42-7.48) (dd, 2H, H<sub>kl</sub>), (δ 7.62) (s, 1H, H<sub>m</sub>), (δ 9.52)

(s, 1H, H<sub>n</sub>), (δ 10.11) (s, 1H, H<sub>o</sub>). FT IR (cm<sup>-1</sup>): 3256 (N-H stretching of secondary amine), 3054 (C-H stretching of aromatic ring), 2954 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2856 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1664 (C=O stretching of amide), 1641 (C=N stretching of triazole ring), 1524 (N-H deformation of pyrimidine ring), 1500 and 1424 (C=C stretching of aromatic ring), 1420 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1413 (C-H symmetrical deformation of CH<sub>3</sub> group), 1334 (C-N stretching), 1221 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1234 (C-O-C stretching), 1013 (C-H in plane deformation of aromatic ring), 834 (C-H out of plane bending of 1,4-disubstitution), 727 (C-Cl stretching), Mass: *m/z* 557; Anal. Calcd. for C<sub>27</sub>H<sub>23</sub>N<sub>7</sub>O<sub>7</sub>: C, 56.81; H, 3.22; N, 18.32; O, 21.15; Found: C, 56.64; H, 3.51; N, 18.13; O, 20.01%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(2-chlorophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4g.** m.p. 184°C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.10) (s, 3H, H<sub>a</sub>), (δ 1.16) (s, 3H, H<sub>b</sub>), (δ 2.52) (d, 1H, H<sub>c</sub>), (δ 6.15) (s, 1H, H<sub>d</sub>), (δ 6.71-6.73) (d, 2H, H<sub>ee</sub>), (δ 6.78-6.80) (d, 1H, H<sub>f</sub>), (δ 7.00-7.04) (t, 2H, H<sub>gg</sub>), (δ 7.10-7.15) (t, 1H, H<sub>h</sub>), (δ 7.20-7.24) (m, 5H, H<sub>i-m</sub>), (δ 7.41-7.51) (dd, 2H, H<sub>no</sub>), (δ 7.52) (s, 1H, H<sub>p</sub>), (δ 9.52) (s, 1H, H<sub>q</sub>), (δ 10.02) (s, 1H, H<sub>r</sub>). FT IR (cm<sup>-1</sup>): 3245 (N-H stretching of secondary amine), 3023 (C-H stretching of aromatic ring), 2917 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2864 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1651 (C=O stretching of amide), 1612 (C=N stretching of triazole ring), 1524 (N-H deformation of pyrimidine ring), 1502 and 1480 (C=C stretching of aromatic ring), 1420 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1405 (C-H symmetrical deformation of CH<sub>3</sub> group), 1356 (C-N stretching), 1254 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1256 (C-O-C stretching), 1021 (C-H in plane deformation of aromatic ring), 828 (C-H out of plane bending of 1,4-disubstitution), 732 (C-Cl stretching), Mass: *m/z* 566; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>ClN<sub>7</sub>O<sub>6</sub>: C, 55.20; H, 3.31; Cl, 6.47; N, 17.89; O, 17.52; Found: C, 54.56; H, 3.21; Cl, 6.20; N, 17.70; O, 17.11%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(4-methoxyphenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4h.** m.p. 185°C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.21) (s, 3H, H<sub>a</sub>), (δ 1.26) (s, 3H, H<sub>b</sub>), (δ 2.36) (d, 1H, H<sub>c</sub>), (δ 6.15) (s, 1H, H<sub>d</sub>), (δ 6.71-6.73) (d, 2H, H<sub>ee</sub>), (δ 6.78-6.80) (d, 1H, H<sub>f</sub>), (δ 7.00-7.04) (t, 2H, H<sub>g</sub>), (δ 7.10-7.15) (t, 1H, H<sub>h</sub>), (δ 7.20-7.24) (m, 5H, H<sub>i,k</sub>), (δ 7.41-7.51) (dd, 2H, H<sub>lm</sub>), (δ 7.52) (s, 1H, H<sub>n</sub>), (δ 9.52) (s, 1H, H<sub>o</sub>), (δ 10.02) (s, 1H, H<sub>p</sub>). FT IR (cm<sup>-1</sup>): 3246 (N-H stretching of secondary amine), 3020 (C-H stretching of aromatic ring), 2926 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2860 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1649 (C=O stretching of amide), 1610 (C=N stretching of triazole ring), 1529 (N-H deformation of pyrimidine ring), 1500 and 1476 (C=C stretching of aromatic ring), 1409 (C-H asymmetrical deformation of CH<sub>3</sub> group), 140 (C-H symmetrical deformation of CH<sub>3</sub> group), 1353 (C-N stretching), 1238 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1250 (C-O-C stretching), 1011 (C-H in plane deformation of aromatic ring), 821 (C-H out of plane bending of 1,4-disubstitution), 756 (C-Cl stretching), Mass: *m/z* 571; Anal. Calcd. for C<sub>28</sub>H<sub>25</sub>N<sub>7</sub>O<sub>7</sub>: C, 57.46; H, 3.89; N, 18.04; O, 20.61; Found: C, 57.34; H, 3.54; N, 18.00; O, 20.53%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(4-bromophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4i.** m.p. 184 °C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.13) (s, 3H, H<sub>a</sub>), (δ 1.19) (s, 3H, H<sub>b</sub>), (δ 2.42) (d, 1H, H<sub>c</sub>), (δ 6.13) (s, 1H, H<sub>d</sub>), (δ 6.54-6.66) (d, 2H, H<sub>ee</sub>), (δ 6.76-6.82) (d, 1H, H<sub>f</sub>), (δ 7.04-7.10) (t, 2H, H<sub>gg</sub>), (δ 7.16-7.36) (dd' dd', 4H, H<sub>hh'-ii'</sub>), (δ 7.48-7.52) (dd, 2H, H<sub>jk</sub>), (δ 7.80) (s, 1H, H<sub>k</sub>), (δ 9.54) (s, 1H, H<sub>m</sub>), (δ 10.13) (s, 1H, H<sub>n</sub>). FT IR (cm<sup>-1</sup>): 3289 (N-H stretching of secondary amine), 3016 (C-H stretching of aromatic ring), 2923 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2824 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1610 (C=O stretching of amide), 1600 (C=N stretching of triazole ring), 1564 (N-H deformation of pyrimidine ring), 1523 and 1446 (C=C stretching of aromatic ring), 1416 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1405 (C-H symmetrical deformation of CH<sub>3</sub> group), 1344 (C-N stretching), 1223 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1201 (C-O-C stretching), 1054 (C-H in plane deformation of aromatic ring), 832 (C-H out of plane bending of 1,4-disubstitution), 730 (C-Br stretching), Mass: *m/z* 619; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>BrN<sub>7</sub>O<sub>6</sub>: C, 50.79; H, 3.06; Br, 13.49; N, 16.45; O, 16.21; Found: C, 50.62; H, 3.00; Br, 13.32; N, 16.20; O, 16.02%.

**7-(4-(2,4-dinitrophenoxy)phenyl)-N-(3-bromophenyl)-4,7-dihydro-5-isopropyl-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide 4j.** m.p. 180 °C; white crystals; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ ppm: (δ 1.13) (s, 3H, H<sub>a</sub>), (δ 1.19) (s, 3H, H<sub>b</sub>), (δ 2.42) (d, 1H, H<sub>c</sub>), (δ 6.32) (s, 1H, H<sub>d</sub>), (δ 6.52-6.64) (d, 2H, H<sub>ee</sub>), (δ 6.74-6.80) (d, 1H, H<sub>f</sub>), (δ 7.00-7.08) (t, 2H, H<sub>gg</sub>), (δ 7.12-7.30) (dd' dd', 4H, H<sub>hh'-ii'</sub>), (δ 7.40-7.42) (dd, 2H, H<sub>jk</sub>), (δ 7.64) (s, 1H, H<sub>l</sub>), (δ 9.67) (s, 1H, H<sub>m</sub>), (δ 10.54) (s, 1H, H<sub>n</sub>). FT IR (cm<sup>-1</sup>): 3254 (N-H stretching of secondary amine), 3021 (C-H stretching of aromatic ring), 2954 (C-H asymmetrical stretching of CH<sub>3</sub> group), 2846 (C-H asymmetrical stretching of CH<sub>3</sub> group), 1602 (C=O stretching of amide), 1584 (C=N stretching of triazole ring), 1512 (N-H deformation of

pyrimidine ring), 1500 and 1456 (C=C stretching of aromatic ring), 1409 (C-H asymmetrical deformation of CH<sub>3</sub> group), 1397 (C-H symmetrical deformation of CH<sub>3</sub> group), 1357 (C-N stretching), 1228 (C-NO<sub>2</sub> symmetrical deformation of NO<sub>2</sub> group), 1211 (C-O-C stretching), 1021 (C-H in plane deformation of aromatic ring), 838 (C-H out of plane bending of 1,4-disubstitution), 724 (C-Br stretching), Mass: *m/z* 619; Anal. Calcd. for C<sub>27</sub>H<sub>22</sub>BrN<sub>7</sub>O<sub>6</sub>: C, 50.69; H, 3.06; Br, 13.49; N, 16.55; O, 16.21; Found: C, 50.54; H, 3.00; Br, 13.17; N, 16.10; O, 16.11%.

#### REFERENCES

- [1] G Fischer; *Adv. Heterocycl. Chem.*, **1993**, 57, 81.
- [2] MAE Shaban; AEA. Morgan, *Adv. Heterocycl. Chem.*, **2000**, 77, 345.
- [3] MAE Shaban; AEA. Morgan, *Adv. Heterocycl. Chem.*, **1999**, 73, 131.
- [4] MAE Shaban; AEA Morgan, *Adv. Heterocycl. Chem.*, **2000**, 75, 243.
- [5] JM Salas; MA Romero; MP Sanchez; M. Quiros, *Coord. Chem. Rev.*, **1999**, 193, 1119.
- [6] E Szlyk; I Łakomska; A Surdykowski; T Głowiak; L Pazderski; J Sitkowski; L.Kozerski, *Inorg. Chim. Acta.*, **2002**, 333, 93.
- [7] M Abul Haj; M Quiros; JM Salas, *Polyhedron*, **2004**, 23, 743.
- [8] M Abul Haj; M Quiros; JM Salas; JA Dobado; J Molina; MG Basallote; MA Manez, *Eur. J. Inorg. Chem.*, **2002**, 811.
- [9] M Biagini-Cingi; AM Manotti-Lanfredi; A Tiripicchio; JG Haasnoot; J Reedijk, *Inorg. Chim. Acta.*, **1985**, 101, 49.
- [10] CO Kappe; WMF Fabian; Semones, *Tetrahedron*, **1997**, 53, 2803.
- [11] M Kidwai; AD Mishra, *Bull. Korean Chem. Soc.*, **2003**, 24, 1038.
- [12] P Biginelli, *Gazz Chim. Ital.*, **1893**, 23, 360.
- [13] CO Kappe; P Rochge, *J. Heterocycl. Chem.*, **1989**, 26, 55. Lin, H.; Ding, J.; Chen, X.; Zhang Z, *Molecules*, **2000**, 5, 1240.
- [14] N Foroughifar; Mobinikhaledi; Fathinejad, *Phosphorus, Sulfur, Silicon*, **2003**, 178, 495.
- [15] MAF Sharaf; FA Abdel; AM Fattah; AMR Khalil. *J. Chem. Research*, **1996**, 354.
- [16] BC O'Reilly; KS Atwal, *Heterocycles*, **1987**, 26, 1158.
- [17] AD Shutalev; EA Kishko. N Sivova; AY Kuzentsov, *Molecules*, **1989**, 3, 100.