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A ONE-POT SEQUENTIAL APPROACH FOR THE CONSTRUCTION OF HIGHLY FUNCTIONALIZED TRIAZOLO[4,3-C]PYRIMIDINE LIBRARY

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Table of Contents

This page	1
Experimental Section.....	2-13
Copies of ¹ H and ¹³ C NMR spectra.....	14-34

Experimental Section

Materials and apparatus:

Thin-layer chromatography was accomplished on 0.2-mm precoated plates of silica gel G60 F²⁵⁴ (Merck). Visualization was made with UV light (254 and 365nm) or with an iodine vapor. ¹H NMR were recorded on a 400 MHz and ¹³C NMR were recorded on a 100 MHz instrument using CDCl₃ and DMSO-d₆ as a solvent on a Bruker AVANCE II spectrometer. Chemical shifts are reported in parts per million relative to tetramethylsilane using the residual solvent signal as the internal reference. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, bs = broad singlet, d = doublet, dd = double doublet, t = triplet, m = multiplet. The ¹³C NMR spectra are proton decoupled. Mass spectra were determined using direct inlet probe on a GCMS-QP 2010 mass spectrometer (Shimadzu). Solvents were evaporated with a BUCHI rotary evaporator. Melting points were measured in open capillaries and are uncorrected. Chemicals were supplied by E. Merck (Germany), Loba Chemie (India) and S. D. Fine Chemicals (India) and used without further purification unless otherwise stated. The solvents were analytical grade and demineralized water was used.

General procedure for the synthesis of 2-(bis(methylthio)methylene)-4-methyl-3-oxo-*N*-(*p*-tolyl)pentanamide 1.¹

To a well-stirred suspension of sodium *tert*-butoxide (2.88 g, 30 mmol) in THF (15 mL) at 0 °C was added CS₂ (0.9 mL, 15 mmol) diluted with 10 mL THF along with *N*-(aryl)-3-oxobutanamide (15 mmol) over a period of 30 min. After completion of the addition, the reaction mixture was stirred at 0 °C for 1.0 h. Appearance of reddish solid in the reaction medium indicated the formation of disodium salt. To this reaction, a solution of methyl iodide (1.86 mL, 30 mmol) in THF (5 mL) was added drop wise within 15 min at 0 °C. The mixture was allowed to warm to room temperature and stirred for 5.0 h, and then poured onto crushed ice (100 g) under stirring. The separated solid was collected by filtration, washed with water (2 × 100 mL), dried in *vacuo* and crystallized from chloroform to furnish the analytically pure products in excellent yield.

General procedure for the synthesis of 4-isopropoxybenzimidamide 2.²

Here starting material thioamide was prepared from corresponding nitrile³. Reaction of 4-isopropoxybenzothioamide with methyl iodide in diethyl ether at RT afford S-methyl thioamide. To a solution of methyl 4-isopropoxybenzimidothioate (5 mmol) in 10 mL of acetonitrile was added ammonium acetate (5 mmol) and stirred at 80 °C for 6 h. After completion of the reaction, solvent was removed in *vacuo* to furnish the analytically pure product in excellent yield, which was used for next step without further purification (yield 92%).

General procedure for the synthesis of 2-substituted-6-isopropyl-4-(methylthio)-*N*-(*p*-tolyl)-1,2-dihydropyrimidine-5-carboxamide **3.²**

To a suspension of 4-isopropoxybenzimidamide **2** (1 mmol) and α -oxo ketene dithioacetals **1** (1 mmol) in dioxane (15mL), dry potassium carbonate (4 mmol) was added, and the reaction mixture was refluxed for appropriate time (**Table 1**) with constant stirring. After completion of the reaction, the reaction mixture was cooled to room temperature and poured in cold water. The separated solid was filtered, washed with water, dried, and used for next step without further purification.

References:

- (1) Savant, M. M.; Pansuriya, A. M.; Bhuva, C. V.; Kapuriya, N.; Patel, A. S.; Audichya, V. B.; Pipaliya, P. V.; Naliapara, Y. T. Water Mediated Construction of Trisubstituted Pyrazoles/Isoxazoles Library Using Ketene Dithioacetals. *J. Comb. Chem.* **2010**, *12*, 176-180.
- (2) Gami, S. P.; Kathrotiya, H. G.; Naliapara, Y. T. One-pot Synthesis of Fully Substituted Pyrimidines Using Amidine and Ketene Dithioacetals as Synthons and Their Antimicrobial Activity. Accepted-2014. DOI 10.1002/jhet.2184.
- (3) Manaka, A.; Sato, M. *Synthetic Commun.* **2005**, *35*, 761-764.

4-isopropoxybenzimidamide 2.

White solid; m.p.162-164 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J*=8.7 Hz, 2H), 7.29 (s, 2H), 6.95 (d, *J*=8.8 Hz), 4.63-4.55 (m, 1H), 1.98 (s, 1H), 1.31 (d, *J*=6.0 Hz, 6H).

2-(4-isopropoxyphenyl)-4-isopropyl-6-(methylthio)-N-(p-tolyl)pyrimidine-5-carboxamide 3.

Yellow solid; m.p.194-196 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 10.75 (s, 1H), 8.34 (d, *J*=8.9 Hz, 2H), 7.57 (d, *J*=8.7 Hz, 2H), 7.19 (d, *J*=8.2 Hz, 2H), 7.09 (d, *J*=8.8 Hz, 2H), 4.79-4.71 (m, 1H), 3.17-3.09 (m, 1H), 2.51 (s, 3H), 2.29 (s, 3H), 1.33-1.30 (m, 12H).

5-(4-isopropoxyphenyl)-7-isopropyl-3-(4-methoxyphenyl)-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide 8a.

Yellow solid; m.p.202-204 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 11.88 (s, 1H), 7.75 (d, *J*=8.1 Hz, 2H), 7.25 (d, *J*=8.6 Hz, 2H), 7.20 (d, *J*=8.1 Hz, 2H), 7.14 (d, *J*=8.5 Hz, 2H), 6.69 (d, *J*=8.5 Hz, 2H), 6.61 (d, *J*=8.5 Hz, 2H), 4.74-4.60 (m, 1H), 4.54-4.44 (m, 1H), 3.75 (s, 3H), 2.36 (s, 3H), 1.41 (d, *J*=6.7 Hz, 6H), 1.30 (d, *J*=5.9 Hz, 6H); ¹³C NMR (400 MHz, Chloroform-*d*) δ 165.25, 161.22, 160.73, 160.62, 151.52, 148.03, 146.94, 136.19, 134.11, 131.30, 131.00, 129.59, 123.29, 120.86, 119.59, 114.75, 113.50, 109.04, 70.16, 55.41, 31.39, 21.94, 21.85, 21.14; MS (*m/z*): 535 (M⁺); Elemental analysis: Calcd. for: C₃₂H₃₃N₅O₃: C, 71.75; H, 6.21; N, 13.07; found: C, 71.38; H, 6.64; N, 12.75.

5-(4-isopropoxyphenyl)-7-isopropyl-N,3-di-p-tolyl-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8b**.

Yellow solid; m.p.180-182 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.68 (s, 1H), 8.41 (d, $J=8.8$ Hz, 2H), 7.63 (s, 1H), 7.48 (d, $J=8.1$ Hz, 3H), 7.17 (d, $J=7.9$ Hz, 3H), 6.96 (d, $J=8.7$ Hz, 3H), 4.71-4.62 (m, 1H), 3.32-3.20 (m, 1H), 2.33 (s, 6H), 1.38 (d, $J=6.0$ Hz, 6H), 1.35 (d, $J=6.5$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 174.77, 164.70, 163.17, 161.28, 157.46, 135.36, 134.71, 130.83, 129.91, 128.45, 125.51, 120.53, 115.66, 70.16, 34.02, 22.19, 21.14; MS (m/z): 519 (M^+); Elemental analysis: Calcd. for: $\text{C}_{32}\text{H}_{33}\text{N}_5\text{O}_2$: C, 73.96; H, 6.40; N, 13.48; found: C, 73.34; H, 6.72; N, 13.93.

3-(2,5-dimethoxyphenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8c**.

Yellow solid; m.p.106-108 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.89 (s, 1H), 7.75 (d, $J=8.1$ Hz, 2H), 7.32-7.26 (m, 3H), 7.21 (d, $J=8.1$ Hz, 2H), 6.85 (d, $J=7.9$ Hz, 1H), 6.59 (d, $J=8.1$ Hz, 2H), 6.30 (d, $J=8.5$ Hz, 1H), 4.69-4.61 (m, 1H), 4.52-4.44 (m, 1H), 3.83 (s, 3H), 3.27 (s, 3H), 2.36 (s, 3H), 1.46 (d, $J=6.1$ Hz, 3H), 1.38 – 1.27 (m, 9H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 165.39, 161.35, 160.32, 153.70, 151.67, 150.06, 148.79, 144.48, 136.24, 134.10, 130.35, 129.60, 123.49, 120.91, 117.87, 117.38, 115.63, 113.92, 110.77, 109.09, 70.17, 56.26, 54.98, 31.46, 22.84, 22.15, 21.86, 21.15, 21.08; MS (m/z): 565 (M^+); Elemental analysis: Calcd. for: $\text{C}_{33}\text{H}_{35}\text{N}_5\text{O}_4$: C, 70.07; H, 6.24; N, 12.38; found: C, 71.64; H, 5.88; N, 12.06.

3-(3,4-dimethoxyphenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8d**.

Yellow solid; m.p.168-170 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.88 (s, 1H), 7.76 (d, $J=8.3$ Hz, 2H), 7.32 (d, $J=8.4$ Hz, 2H), 7.22 (d, $J=8.4$ Hz, 2H), 6.85-6.77 (m, 2H), 6.70-6.62 (m, 3H), 4.73-4.62 (m, 1H), 4.56-4.45 (m, 1H), 3.85 (s, 3H), 3.72 (s, 3H), 2.37 (s, 3H) 1.42 (d, $J=6.6$ Hz, 6H), 1.32 (d, $J=6.1$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 165.17, 161.16, 160.74, 151.62, 150.37, 148.51, 147.90, 146.91, 136.16, 134.13, 131.27, 130.30, 129.58, 123.53, 123.07, 120.80, 119.57, 114.74, 112.46, 110.39, 109.01, 70.20, 56.04, 55.97, 31.38, 21.94, 21.82, 21.13; MS (m/z): 565 (M^+); Elemental analysis: Calcd. for: $\text{C}_{33}\text{H}_{35}\text{N}_5\text{O}_4$: C, 70.07; H, 6.24; N, 12.38; found: C, 69.68; H, 6.46; N, 11.97.

3-(4-(dimethylamino)phenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8e**.

Yellow solid; m.p.250-252 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.99 (s, 1H), 7.76 (d, $J=7.9$ Hz, 2H), 7.27 (d, $J=7.9$ Hz, 2H), 7.20 (d, $J=7.1$ Hz, 2H), 7.04 (d, $J=7.9$ Hz, 2H), 6.60 (d, $J=7.6$ Hz, 2H), 6.42 (d, $J=7.9$ Hz, 2H), 4.67 (s, 1H), 4.48 (s, 1H), 2.92 (s, 6H), 2.36 (s, 3H), 1.44-1.25 (m, 12H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 164.88, 161.40, 160.41, 151.25, 150.92, 148.27, 147.77, 136.28, 134.00, 131.39, 130.51, 129.56, 123.43, 120.85, 114.55, 114.05, 110.99, 108.86, 69.97, 40.19, 31.32, 21.95, 21.87, 21.14; MS (m/z): 548 (M^+); Elemental analysis: Calcd. for: $\text{C}_{33}\text{H}_{36}\text{N}_6\text{O}_2$: C, 72.24; H, 6.61; N, 15.32; found: C, 72.71; H, 6.18; N, 14.85.

3-(4-fluorophenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8f**.

Yellow solid; m.p.180-182 °C ; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.76 (s, 1H), 7.74 (d, $J=8.2$ Hz, 2H), 7.17-7.27 (m, 6H), 6.88 (t, 2H), 6.62 (d, $J=8.5$ Hz, 2H), 4.71-4.58 (m, 1H), 4.55-4.44 (m, 1H), 2.35 (s, 3H), 1.40 (d, $J=6.8$ Hz, 6H), 1.31 (d, $J=6.0$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 165.38, 164.46, 162.14, 160.87, 151.67, 147.77, 146.03, 136.05, 134.15, 131.54, 131.21, 129.55, 123.47, 123.07, 120.79, 115.23, 114.87, 109.15, 70.27, 31.40, 21.89, 21.78, 21.09; MS (m/z): 523 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{30}\text{FN}_5\text{O}_2$: C, 71.11; H, 5.78; N, 13.38; found: C, 76.79; H, 5.32; N, 13.68.

3-(2-chlorophenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8g**.

Yellow solid; m.p.198-200 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.75 (s, 1H), 7.75 (d, $J=8.1$ Hz, 2H), 7.51 (d, $J=7.7$ Hz, 1H), 7.29-7.25 (m, 3H), 7.21 (d, $J=7.7$ Hz, 2H), 7.09 (d, $J=7.5$ Hz, 1H), 6.55 (d, $J=8.4$ Hz, 2H), 4.69-4.61 (m, 1H), 4.50-4.43 (m, 1H), 2.36 (s, 3H), 1.43 (d, $J=6.2$ Hz, 3H), 1.37 (d, $J=6.2$ Hz, 3H), 1.31-1.25 (m, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 165.61, 160.92, 160.18, 151.41, 148.20, 144.12, 135.91, 134.49, 134.05, 131.96, 131.38, 131.06, 129.44, 129.29, 127.49, 126.77, 122.54, 120.78, 114.10, 109.23, 70.00, 31.36, 22.31, 21.88, 21.75, 21.22, 20.99; MS (m/z): 540 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{30}\text{ClN}_5\text{O}_2$: C, 68.94; H, 5.60; N, 12.97; found: C, 68.38; H, 5.86; N, 12.45.

3-(4-bromophenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8h**.

Yellow solid; m.p.226-228 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.77 (s, 1H), 7.76 (d, $J=8.4$ Hz, 2H), 7.28-7.25 (m, 3H), 7.24-7.20 (m, 4H), 6.68-6.65 (m, 2H), 4.70-4.67 (m, 1H), 4.57-4.50 (m, 1H), 2.38 (s, 3H), 1.42 (d, $J=6.8$ Hz, 6H), 1.35 (d, $J=6.0$ Hz, 6H). ^{13}C NMR (400 MHz, Chloroform-*d*) δ 174.77, 164.70, 163.16, 161.28, 157.46, 155.32, 135.36, 134.71, 130.83, 130.65, 130.55, 130.19, 130.13, 129.91, 128.45, 125.51, 120.53, 115.66, 70.16, 34.01, 22.19, 21.14; MS (m/z): 584 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{30}\text{BrN}_5\text{O}_2$: C, 63.70; H, 5.17; N, 11.98; found: C, 63.23; H, 4.87; N, 11.54.

3-(2-bromophenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8i**.

Yellow solid; m.p.230-232 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.78 (s, 1H), 7.77 (d, $J=8.0$ Hz, 2H), 7.46 (d, 1H), 7.35-7.28 (m, 4H), 7.26-7.17 (m, 3H), 6.56 (d, $J=8.4$ Hz, 2H), 4.73-4.63 (m, 1H), 4.53-4.43 (m, 1H), 2.38 (s, 3H), 1.45 (d, $J=6.7$ Hz, 3H), 1.40 (d, $J=6.3$ Hz, 3H), 1.34 – 1.27 (m, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 165.65, 160.96, 160.20, 151.36, 148.22, 145.25, 135.97, 134.08, 132.56, 132.38, 131.38, 131.23, 129.48, 127.24, 124.55, 122.65, 120.82, 114.17, 114.08, 109.31, 70.05, 31.40, 22.28, 21.93, 21.80, 21.35, 21.04; MS (m/z): 584 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{30}\text{BrN}_5\text{O}_2$: C, 63.70; H, 5.17; N, 11.98; found: C, 63.94; H, 6.04; N, 11.54.

3-(3-bromophenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8j**.

Yellow solid; m.p.212-214 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.63 (s, 1H), 7.66 (d, $J=8.0$ Hz, 2H), 7.33 (d, $J=8.0$ Hz, 1H), 7.24 (d, $J=8.0$ Hz, 1H), 7.20-7.11 (m, 4H), 7.03 (t, 1H), 6.56 (d, $J=8.6$ Hz, 2H), 4.61-4.54 (m, 1H), 4.47-4.40 (m, 1H), 2.27 (s, 3H), 1.32 (d, $J=6.4$ Hz, 6H), 1.25 (d, $J=6.0$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 165.71, 160.98, 151.89, 147.80, 145.60, 136.06, 134.25, 132.77, 132.68, 131.03, 129.62, 129.04, 128.10, 123.11, 121.91, 120.89, 114.97, 109.29, 70.36, 31.48, 21.01, 21.94, 21.15; MS (m/z): 584 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{30}\text{BrN}_5\text{O}_2$: C, 63.70; H, 5.17; N, 11.98; found: C, 63.92; H, 5.28; N, 12.24.

3-(4-cyanophenyl)-5-(4-isopropoxyphenyl)-7-isopropyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8k**.

Yellow solid; m.p.238-240 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.59 (s, 1H), 7.72 (d, $J=8.3$ Hz, 2H), 7.48 (d, $J=8.2$ Hz, 2H), 7.37 (d, $J=8.2$ Hz, 2H), 7.26 (d, $J=8.7$ Hz, 2H), 7.20 (d, $J=8.0$ Hz, 2H), 6.62 (d, $J=8.3$ Hz, 2H), 4.66-4.58(m, 1H), 4.54-4.47 (m, 1H), 2.36 (s, 3H), 1.40 (d, $J=6.5$ Hz, 6H), 1.33 (d, $J=6.2$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 177.36, 165.95, 164.82, 163.96, 162.34, 151.14, 148.90, 138.48, 137.65, 134.29, 133.76, 133.10, 132.25, 132.16, 130.08, 126.10, 122.72, 121.48, 121.03, 118.79, 115.44, 32.44, 21.89, 20.16, 19.43; MS (m/z): 519 (M^+); Elemental analysis: Calcd. for: $\text{C}_{32}\text{H}_{30}\text{N}_6\text{O}_2$: C, 72.43; H, 5.70; N, 15.84; found: C, 72.16; H, 5.94; N, 15.42

5-(4-isopropoxyphenyl)-7-isopropyl-3-(4-nitrophenyl)-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8l**.

Yellow solid; m.p.258-260 °C ; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.60 (s, 1H), 8.05 (d, $J=7.7$ Hz, 2H), 7.73 (d, $J=7.6$ Hz, 2H), 7.45 (d, $J=7.7$ Hz, 2H), 7.28 (d, $J=7.9$, 8.1 Hz, 4H), 7.29 (d, $J=7.9$ Hz, 2H), 7.21 (d, $J=7.9$ Hz, 2H), 4.70-4.60 (m, 1H), 4.51-4.40 (m, 1H), 2.37 (s, 3H), 1.41 (d, $J=5.5$ Hz, 6H), 1.27 (d, $J=5.9$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 166.23, 161.22, 160.74, 152.36, 147.99, 147.52, 145.08, 135.95, 134.46, 133.40, 131.14, 130.37, 129.69, 123.04, 120.88, 115.16, 109.45, 70.46, 31.61, 21.96, 21.71, 21.17; MS (m/z): 550 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{30}\text{N}_6\text{O}_4$: C, 67.62; H, 5.49; N, 15.26; found: C, 67.18; H, 5.21; N, 14.83.

5-(4-isopropoxyphenyl)-7-isopropyl-3-(2-nitrophenyl)-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8m**.

Yellow solid; m.p.242-244 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.50 (s, 1H), 7.84 (d, $J=8.1$ Hz, 2H), 7.73-7.53 (m, 5H), 7.48 (t, 1H), 7.13 (d, $J=8.1$ Hz, 2H), 7.06 (d, $J=8.1$ Hz, 2H), 4.58-4.50 (m, 1H), 4.43- 4.35 (m, 1H), 2.28 (s, 3H), 1.34-1.28 (m, 6H), 1.22 (d, $J=5.9$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 165.88, 160.97, 160.27, 151.63, 147.98, 147.00, 143.84, 136.00, 134.31, 133.92, 133.31, 131.35, 130.90, 129.62, 124.88, 124.06, 122.43, 120.98, 114.84, 110.08, 70.24, 31.58, 21.96, 21.16; MS (m/z): 550 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{30}\text{N}_6\text{O}_4$: C, 67.62; H, 5.49; N, 15.26; found: C, 67.22; H, 5.11; N, 15.81.

5-(4-isopropoxyphenyl)-7-isopropyl-3-phenyl-N-(p-tolyl)-[1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamide **8n**.

Yellow solid; m.p. 186-188 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 11.77 (s, 1H), 8.48-8.22 (m, 4H), 7.52-7.36 (m, 3H), 7.22-7.02 (m, 4H), 6.89 (d, $J=8.7$ Hz, 2H), 4.66-4.54 (m, 1H), 3.26-3.14 (m, 1H), 2.28 (s, 3H), 1.31 (d, $J=6.1$ Hz, 6H), 1.29 (d, $J=6.7$ Hz, 6H); ^{13}C NMR (400 MHz, Chloroform-*d*) δ 174.81, 164.72, 163.12, 161.29, 157.46, 135.38, 134.71, 130.83, 129.93, 129.62, 128.43, 125.50, 120.51, 115.66, 70.16, 34.03, 22.20, 21.16; MS (m/z): 505 (M^+); Elemental analysis: Calcd. for: $\text{C}_{31}\text{H}_{31}\text{N}_5\text{O}_2$: C, 73.64; H, 6.18; N, 13.85; found: C, 73.10; H, 5.79; N, 14.21.

¹H NMR Spectrum of Compound 2:

¹H NMR Spectrum of Compound 3:

Mass spectrum of compound 8a:

Line#:1 R.Time:4.2(Scan#:560)

MassPeaks:280

RawMode:Averaged 3.1-6.0(394-819) BasePeak:43.050(26007)

BG Mode:None Group 1 - Event 1

¹H and ¹³C NMR Spectrum of Compound 8b:

¹H NMR

¹³C NMR

¹H and ¹³C NMR Spectrum of Compound 8c:

¹H NMR

¹³C NMR

Mass spectrum of compound 8c:

Line#:1 R.Time:3.4(Scan#:352)

MassPeaks:285

RawMode:Averaged 2.6-4.5(250-477) BasePeak:565.050(234749)

BG Mode:None Group 1 - Event 1

¹H and ¹³C NMR Spectrum of Compound 8d:

¹H NMR

¹³C NMR

¹H and ¹³C NMR Spectrum of Compound 8e:

¹H NMR

¹³C NMR

¹H and ¹³C NMR Spectrum of Compound 8f:

¹H NMR

¹³C NMR

Mass Spectrum of compound 8f:

Line#:1 R.Time:4.4(Scan#:518)

MassPeaks:205

RawMode:Averaged 2.0-6.0(146-749) BasePeak:229.100(4603)

BG Mode:None Group 1 - Event 1

¹H and ¹³C NMR Spectrum of Compound 8g:

¹H NMR

¹³C NMR

Mass spectrum of Compound 8g:

Line#:1 R.Time:4.4(Scan#:470)

MassPeaks:351

RawMode:Averaged 2.9-6.1(290-670) BasePeak:107.050(13942)

BG Mode:None Group 1 - Event 1

¹H and ¹³C NMR Spectrum of Compound 8h:

¹H NMR

¹³C NMR

Mass spectrum of Compound 8h:

Line#:1 R.Time:4.0(Scan#:424)

MassPeaks:436

RawMode:Averaged 2.7-5.9(266-643) BasePeak:107.000(33766)

BG Mode:None Group 1 - Event 1

¹H and ¹³C NMR Spectrum of Compound 8i:

¹H NMR

¹³C NMR

Mass spectrum of Compound 8i:

Line#:1 R.Time:4.2(Scan#:560)

MassPeaks:422

RawMode:Averaged 3.3-5.7(421-776) BasePeak:43.050(51119)

BG Mode:None Group 1 - Event 1

¹H and ¹³C NMR Spectrum of Compound 8j:

¹H NMR

¹³C NMR

¹H and ¹³C NMR Spectrum of Compound 8k:

¹H NMR

¹³C NMR

¹H and ¹³C NMR Spectrum of Compound 8l:

¹H NMR

¹³C NMR

¹H and ¹³C NMR Spectrum of Compound 8m:

¹H NMR

¹³C NMR

¹H and ¹³C NMR Spectrum of Compound 8n:

¹H NMR

¹³C NMR