Base-Catalyzed, Efficient Synthesis of 5-Substituted 3,6-Dihydro-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones

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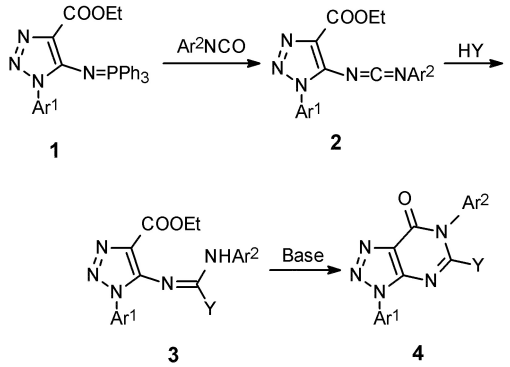
Abstract: The carbodiimides **2**, obtained from aza-Wittig reactions of iminophosphorane **1** with aromatic isocyanates, reacted with secondary amines or ROH to give 5-dialkylamino or 5-alkoxy 7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4** in the presence of a catalytic amount of EtONa in a mixed solvent (CH_2Cl_2–ROH). Reactions of **2** with phenols in presence of catalytic potassium carbonate in MeCN gave 5-aryloxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4** in satisfactory yields.

Key words: pyrimidines, imides, cyclizations, aza-Wittig reactions, heterocycles, guanines

7*H*-1,2,3-Triazolo[4,5-*d*]pyrimidin-7-ones, which are also named as 8-azaguanines, are of great importances because of their structural similarity with guanines. Some derivatives of them have shown remarkable biological (antiguanine) properties such as antitumor, antiviral, and anti-HIV activities,[1–5] whereas others exhibited good fungicidal activities.[6] The methods described for the preparation of this ring system either involves reaction of properly substituted diaminopyrimidines with sodium nitrate and acetic acid, or reaction of aminotriazolecarbonamides with orthoformate, or cyclization of 5-acetamido-4-ethoxycarbonyl- 1,2,3-triazoles with amine in the presence of phosphorus pentoxide.[6–12] However, these methods often require relatively harsh acid, dehydrating conditions or heating at high temperature, and there is no report of a generally useful synthesis of 5-amino or 5-aryl(alk)oxy substituted 7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones starting from easily accessible 5-amino-4-ethoxycarbonyl-1,2,3-triazoles.

Recently we have been interested in the synthesis of quinazolinones, thienopyrimidinones and imidazolinones via aza-Wittig reaction of α or β ethoxycarbonyl iminophosphorane with aromatic isocyanate and subsequent reaction with various nucleophiles under mild conditions.[13–17] Here we wish to report a base-catalyzed, efficient approach to 5-substituted 7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones.

It was reported that iminophosphorane **1** reacted with aromatic isocyanates to give carbodiimides **2**, which were allowed to react with secondary amines to provide guanidines **3**.[18] Our recent results on synthesis of fused pyrimidinones[13,15] imply that guanidines **3** may be transformed into 7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4** in the presence of a catalytic amount of sodium ethoxide. However, when treated with sodium ethoxide in EtOH at room temperature, the guanidines **3** were recovered unchanged, probably due to the low solubility of **3** in EtOH. In refluxing EtOH in the presence of EtONa, a complex mixture resulted, probably owning to the instability of the product at reflux temperature in strong basic conditions. We found that when a mixed solvent (CH_2Cl_2–EtOH) was used in the presence of a catalytic amount of sodium ethoxide, compounds **3** were converted easily to 5-dialkylamino-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4** (Y = NR^1R^2) in satisfactory yields at room temperature. This may be due to the good solubility of **3** in the mixed solvent. It is noteworthy that the isolated yield of **4** was good even when Y is a bulky diisopropylamino group. The results are listed in Table 1.



Scheme 1

When carbodiimide **2** was reacted with ROH, only the urea-type product **3** was obtained.[18,19] However, 5-alkoxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4** (Y = OR) were obtained from **3** in satisfactory yields in the presence of catalytic amount of RONa by using the mixed solvent (CH_2Cl_2–ROH). The reaction of carbodiimide **2** with phenols in the presence of a catalytic amount of potassium carbonate produced 5-aryloxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4** (Y = OAr) directly in good yields when MeCN was used as solvent. The reaction is relatively insensitive to the presence or absence of substituents on the phenols and the cyclization can be completed smoothly at 40–50 °C. The facile cyclization

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Table 1 Preparation of 5-Substituted 7*H*-1,2,3-Triazolo[4,5-*d*]pyrimidin-7-ones **4**

	Ar[1]	Ar[2]	Y	Yield (%)[a]
4a	Ph	Ph	NEt_2	84
4b	Ph	Ph	$N(Pr)_2$	80
4c	Ph	Ph	$N(n\text{-}Bu)_2$	87
4d	Ph	Ph		88
4e	Ph	Ph	$N(i\text{-}Bu)_2$	78
4f	Ph	Ph	NMe(Ph)	85
4g	Ph	Ph	$N(i\text{-}Pr)_2$	73
4h	Ph	4-ClC_6H_4	NEt_2	86
4i	4-ClC_6H_4	Ph	NEt_2	81
4j	4-ClC_6H_4	Ph	NMe(Ph)	75
4k	Ph	Ph	OMe	86
4l	Ph	Ph	OEt	82
4m	Ph	Ph	$OCH_2C{\equiv}CH$	71
4n	Ph	Ph	$OCH_2CH{=}CH_2$	73
4o	Ph	4-ClC_6H_4	OEt	83
4p	4-ClC_6H_4	Ph	OEt	87
4q	Ph	Ph	4-$MeOC_6H_4O$	81
4r	Ph	Ph	4-MeC_6H_4O	74
4s	4-ClC_6H_4	3-MeC_6H_4	4-$MeOC_6H_4O$	82
4t	4-ClC_6H_4	3-MeC_6H_4	4-MeC_6H_4O	84
4u	4-ClC_6H_4	3-MeC_6H_4	PhO	77
4v	4-ClC_6H_4	Ph	4-ClC_6H_4O	72

[a] Isolated yields based on iminophosphorane **1**.

condition (K_2CO_3 catalyzed) in this case is probably due to the more acidic NHAr in intermediate **3** when Y is OAr.

In conclusion, we have developed an efficient synthesis of 5-substituted 7*H*-1,2,3-triazolo[4,5-*d*] pyrimidin-7-ones via aza-Wittig reactions. Due to the mild reaction conditions, good yields, easily accessible starting material and straightforward product isolation, we think that the versatile synthetic approach discussed here in many cases compares favorably with other existing methods.

Mps were uncorrected. MS spectra were measured on a Finnigan Trace MS spectrometer. IR spectra were recorded on a PE-983 infrared spectrometer as KBr pellets with absorption in cm^{-1}. NMR spectra were recorded in $CDCl_3$ on a Varian Mercury 400 spectrometer and resonances are given in ppm (δ) relative to TMS. Elemental analyses were taken on a Vario EL III elemental analysis instrument. Petroleum ether refers to the fraction with bp 60–90 °C.

5-Dialkylamino-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones (4)

To a solution of iminophosphorane **1**[20,21] (2 mmol) in anhyd CH_2Cl_2 (15 mL) was added aromatic isocyanate (2 mmol) under nitrogen at r.t. After the reaction mixture was allowed to stand for 24–30 hours at 0–5 °C, the solvent was removed under reduced pressure and Et_2O–petroleum ether (1:2; 20 mL) was added to precipitate the triphenylphosphine oxide. After filtration, the solvent was removed to give carbodiimide **2**, which was used directly without further purification. To the solution of **2** prepared above in CH_2Cl_2 (15 mL) was added dialkylamine (2 mmol). After the reaction mixture was allowed to stand for 0.5–6 h, the solution was condensed and anhyd EtOH–CH_2Cl_2 (4:1, 10 mL) with several drops of EtONa in EtOH was added. The mixture was stirred for 1–6 h at r.t. The solution was concentrated under reduced pressure and the residue was recrystallized from EtOH to give the 5-dialkylamino-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4**.

5-Diethylamino-3,6-dihydro-3,6-diphenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4a)

White crystals; mp 182–183 °C.

IR (KBr): 1719 (C=O), 1520, 1354, 1080 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 0.88 (t, *J* = 7.2 Hz, 6 H), 3.20 (q, *J* = 7.2 Hz, 4 H), 7.32–8.19 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 11.96 (2), 45.33 (2), 120.68 (2), 125.97, 127.75, 128.33, 128.80 (2), 129.12 (4), 136.18, 137.65, 147.74, 156.67, 158.28.

MS: *m*/*z* (%) = 360 (97) [M^+], 332 (80), 303 (45), 200 (13), 77 (100).

Anal. Calcd for $C_{20}H_{20}N_6O$: C, 66.65; H, 5.59; N, 23.32. Found: C, 66.87; H, 5.41; N, 23.46.

3,6-Dihydro-3,6-diphenyl-5-di(propyl)amino-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4b)

White crystals; mp 142–144 °C.

IR (KBr): 1726 (C=O), 1521, 1370, 1038 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 0.75 (t, *J* = 7.2 Hz, 6 H), 1.29–1.35 (m, 4 H), 3.06 (t, *J* = 7.6 Hz, 4 H), 7.32–8.20 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 11.15 (2), 20.39 (2), 53.23 (2), 120.63 (2), 125.86, 127.74, 128.42, 128.67 (2), 129.11 (4), 136.24, 137.50, 147.75, 156.64, 158.14.

MS: *m*/*z* (%) = 388 (73) [M^+], 360 (25), 318 (17), 289 (100), 77 (68).

Anal. Calcd for $C_{22}H_{24}N_6O$: C, 68.02; H, 6.23; N, 21.63. Found: C, 68.26; H, 6.20; N, 21.77.

5-Di(*n*-butyl)amino-3,6-dihydro-3,6-diphenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4c)

White crystals; mp 138–140 °C.

IR (KBr): 1725 (C=O), 1528, 1368, 1030 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 0.85 (t, *J* = 7.2 Hz, 6 H), 1.12–1.30 (m, 8 H), 3.10 (t, *J* = 7.6 Hz, 4 H), 7.31–8.21 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.62 (2), 20.06 (2), 29.14 (2), 51.40 (2), 120.69 (2), 125.90, 127.77, 128.36, 128.71, 129.09 (2), 129.14 (4), 136.26, 137.57, 147.78, 156.68, 158.22.

MS: *m*/*z* (%) = 416 (85) [M^+], 388 (29), 331 (35), 289 (66), 77 (100).

Anal. Calcd for $C_{24}H_{28}N_6O$: C, 69.21; H, 6.78; N, 20.18. Found: C, 69.16; H, 6.54; N, 20.24.

3,6-Dihydro-3,6-diphenyl-5-(1-piperidinyl)-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4d)

White crystals; mp 189–191 °C.

IR (KBr): 1727 (C=O), 1518, 1348, 1252, 1026 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 1.29–1.47 (m, 6 H), 3.21 (q, *J* = 5.6 Hz, 4 H), 7.35–8.19 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 23.68, 24.50 (2), 49.97 (2), 120.69 (2), 126.32, 127.78, 128.13, 128.52 (2), 128.90 (2), 129.11 (2), 136.09, 137.37, 147.54, 156.36, 158.81.

MS: *m*/*z* (%) = 372 (76) [M^+], 344 (55), 315 (16), 212 (32), 77 (100).

Anal. Calcd for $C_{21}H_{20}N_6O$: C, 67.73; H, 5.41; N, 22.57. Found: C, 67.58; H, 5.47; N, 22.75.

5-Di(isobutyl)amino-3,6-dihydro-3,6-diphenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4e)
White crystals; mp 217–219 °C.

IR (KBr): 1725 (C=O), 1523, 1367, 1033 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 0.82 (t, *J* = 6.8 Hz, 12 H), 1.88–1.93 (m, 2 H), 2.92 (d, *J* = 6.8 Hz, 4 H), 7.33–8.21 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.19 (4), 27.62 (2), 60.14 (2), 120.81, 125.75, 127.84, 128.44 (2), 128.65, 129.23 (4), 136.39, 137.30, 147.91, 156.65, 157.80.

MS: *m*/*z* (%) = 416 (67) [M^+], 345 (30), 288 (100), 77 (74).

Anal. Calcd for $C_{24}H_{28}N_6O$: C, 69.21; H, 6.78; N, 20.18. Found: C, 69.04; H, 6.84; N, 20.42.

3,6-Dihydro-3,6-diphenyl-5-(*N*-phenyl-*N*-methylamino)-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4f)
White crystals; mp 244–246 °C.

IR (KBr): 1721 (C=O), 1532, 1387, 1066 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 3.37 (s, 3 H), 6.58–8.28 (m, 15 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 43.31, 121.01 (2), 125.59 (2), 126.10, 126.85, 127.61, 128.08, 128.30 (2), 128.79 (2), 129.29 (4), 136.16, 136.27, 145.70, 147.53, 156.34, 157.66.

MS: *m*/*z* (%) = 394 (98) [M^+], 365 (100), 289 (64), 234 (88), 103 (97).

Anal. Calcd for $C_{23}H_{18}N_6O$: C, 70.04; H, 4.60; N, 21.31. Found: C, 70.27; H, 4.71; N, 21.06.

3,6-Dihydro-3,6-diphenyl-5-di(isopropyl)amino-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4g)
White crystals; mp 228–230 °C.

IR (KBr): 1721 (C=O), 1524, 1364, 1027 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 1.10 (d, *J* = 6.8 Hz, 12 H), 3.62–3.69 (m, 2 H), 7.29–8.12 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.14 (4), 50.63 (2), 121.58 (2), 126.27, 128.02, 128.27, 129.08 (2), 129.17 (2), 129.28 (2), 136.06, 138.85, 147.70, 157.38, 157.60.

MS: *m*/*z* (%) = 388 (29) [M^+], 345 (15), 317 (64), 303 (28), 42 (100).

Anal. Calcd for $C_{22}H_{24}N_6O$: C, 68.02; H, 6.23; N, 21.63. Found: C, 68.18; H, 6.01; N, 21.85.

6-(4-Chlorophenyl)-5-diethylamino-3,6-dihydro-3-phenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4h)
White crystals; mp 231–232 °C.

IR (KBr): 1708 (C=O), 1541, 1353, 1090 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 0.93 (t, *J* = 7.2 Hz, 6 H), 3.21 (q, *J* = 7.2 Hz, 4 H), 7.28–8.17 (m, 9 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.17 (2), 45.41 (2), 120.89 (2), 125.99, 127.98, 129.25 (2), 129.46 (2), 130.19 (2), 134.41, 136.11, 136.18, 147.75, 156.52, 158.15.

MS: *m*/*z* (%) = 396/394 (32/96) [M^+], 366 (45), 337 (35), 136 (44), 76 (100).

Anal. Calcd for $C_{20}H_{19}ClN_6O$: C, 60.84; H, 4.85; N, 21.28. Found: C, 60.78; H, 4.81; N, 21.16.

3-(4-Chlorophenyl)-5-diethylamino-3,6-dihydro-6-phenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4i)
White crystals; mp 234–235 °C.

IR (KBr): 1716 (C=O), 1520, 1351, 1034 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 0.88 (t, *J* = 7.2 Hz, 6 H), 3.21 (q, *J* = 7.2 Hz, 4 H), 7.27–8.18 (m, 9 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.09 (2), 45.49 (2), 121.91 (2), 126.10, 128.57, 128.89 (2), 129.32 (2), 129.44 (2), 133.52, 134.91, 137.71, 147.89, 156.66, 158.52.

MS: *m*/*z* (%) = 396/394 (1/3) [M^+], 366 (2), 287 (2), 137 (84), 77 (100).

Anal. Calcd for $C_{20}H_{19}ClN_6O$: C, 60.84; H, 4.85; N, 21.28. Found: C, 60.95; H, 4.74; N, 21.34.

3-(4-Chlorophenyl)-3,6-dihydro-6-phenyl-5-(*N*-phenyl-*N*-methylamino)-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4j)
White crystals; mp 275–277 °C.

IR (KBr): 1722 (C=O), 1521, 1392, 1091 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 3.37 (s, 3 H), 6.59–8.26 (m, 14 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 43.40, 122.15 (2), 125.70 (2), 126.30, 126.92, 127.76, 128.43 (2), 128.85 (2), 129.40 (2), 129.55 (2), 133.80, 134.83, 136.28, 145.68, 147.61, 156.26, 157.89.

MS: *m*/*z* (%) = 430/428 (9/25) [M^+], 400 (16), 365 (7), 234 (38), 77 (100).

Anal. Calcd for $C_{23}H_{17}ClN_6O$: C, 64.41; H, 4.00; N, 19.60. Found: C, 64.67; H, 4.18; N, 19.34.

5-Alkoxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones (4)
To **2** prepared above was added ROH (8 mL). After urea-type compound **3** was precipitated from the reaction mixture, CH_2Cl_2 (2 mL) was added to dissolve the solid and then RONa in ROH (several drops) was added. The mixture was stirred for 6 h at r.t. The solution was condensed and the precipitate was collected to give 5-alkoxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4**.

3,6-Dihydro-3,6-diphenyl-5-methoxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4k)
White crystals; mp 203–204 °C.

IR (KBr): 1721 (C=O), 1557, 1345, 1035 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ = 4.03 (s, 3 H), 7.24–8.15 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 56.89, 121.33 (2), 127.25, 128.15 (2), 128.48, 129.20, 129.40 (2), 129.45 (2), 134.08, 135.80, 146.89, 155.39, 157.41.

MS: *m*/*z* (%) = 319 (100) [M^+], 290 (21), 276 (36), 145 (83), 77 (88).

Anal. Calcd for $C_{17}H_{13}N_5O_2$: C, 63.94; H, 4.10; N, 21.93. Found: C, 63.88; H, 4.04; N, 22.07.

3,6-Dihydro-3,6-diphenyl-5-ethoxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4l)
White crystals; mp 217–219 °C.

IR (KBr): 1725 (C=O), 1555, 1329, 1033 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.29 (t, *J* = 7.2 Hz, 3 H), 4.51 (q, *J* = 7.2 Hz, 2 H), 7.23–8.14 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.78, 66.39, 121.31 (2), 127.24, 128.12 (2), 128.42, 129.06, 129.37 (4), 134.21, 135.84, 147.04, 155.50, 156.86.

MS: *m*/*z* (%) = 333 (100) [M$^+$], 276 (70), 248 (23), 145 (60), 77 (68).

Anal. Calcd for $C_{18}H_{15}N_5O_2$: C, 64.86; H, 4.54; N, 21.01. Found: C, 64.63; H, 4.69; N, 21.07.

3,6-Dihydro-3,6-diphenyl-5-propargyloxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4m)
White crystals; mp 226–227 °C.

IR (KBr): 3295, 2131 (C≡C), 1724 (C=O), 1557, 1372 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.55 (s, 1 H), 5.01 (s, 2 H), 7.25–8.17 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 57.13, 76.25, 76.39, 121.41 (2), 127.47, 128.18 (2), 128.60, 129.38, 129.47 (2), 129.54 (2), 133.74, 135.75, 146.45, 155.25, 155.93.

MS: *m*/*z* (%) = 343 (50) [M$^+$], 276 (41), 145 (100), 129 (30), 77 (67).

Anal. Calcd for $C_{19}H_{13}N_5O_2$: C, 66.47; H, 3.82; N, 20.40. Found: C, 66.53; H, 3.76; N, 20.27.

5-Allyloxy-3,6-dihydro-3,6-diphenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4n)
White crystals; mp 203–205 °C.

IR (KBr): 1718 (C=O), 1553, 1367, 769 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.93 (d, *J* = 5.2 Hz, 2 H), 5.13–5.23 (m, 2 H), 5.83–5.93 (m, 1 H), 7.24–8.12 (m, 10 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 70.18, 118.91, 121.44 (2), 127.34, 128.15 (2), 128.53, 129.22, 129.42 (2), 129.47 (2), 130.44, 134.11, 135.80, 146.90, 155.45, 156.56.

MS: *m*/*z* (%) = 345 (41) [M$^+$], 316 (15), 276 (39), 145 (100), 77 (77).

Anal. Calcd for $C_{19}H_{15}N_5O_2$: C, 66.08; H, 4.38; N, 20.28. Found: C, 66.23; H, 4.15; N, 20.17.

6-(4-Chlorophenyl)-3,6-dihydro-5-ethoxy-3-phenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4o)
White crystals; mp 245–246 °C.

IR (KBr): 1719 (C=O), 1558, 1325, 1091 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.31 (t, *J* = 7.2 Hz, 3 H), 4.52 (q, *J* = 7.2 Hz, 2 H), 7.18–8.12 (m, 9 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.84, 66.63, 121.40 (2), 127.11, 128.54, 129.43 (2), 129.60 (2), 129.69 (2), 132.68, 135.15, 135.79, 147.02, 155.34, 156.60.

MS: *m*/*z* (%) = 369/367 (32/92) [M$^+$], 310 (29), 282 (16), 124 (30), 76 (100).

Anal. Calcd for $C_{18}H_{14}ClN_5O_2$: C, 58.78; H, 3.84; N, 19.04. Found: C, 58.83; H, 3.75; N, 19.02.

3-(4-Chlorophenyl)-3,6-dihydro-5-ethoxy-6-phenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4p)
White crystals; mp 199–200 °C.

IR (KBr): 1731 (C=O), 1550, 1332, 1073 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.29 (t, *J* = 7.2 Hz, 3 H), 4.51 (q, *J* = 7.2 Hz, 2 H), 7.22–8.12 (m, 9 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.70, 66.49, 122.24 (2), 127.16, 128.02 (2), 129.01, 129.28 (2), 129.47 (2), 134.03 (2), 134.29, 146.95, 155.26, 156.96.

MS: *m*/*z* (%) = 369/367 (25/72) [M$^+$], 311 (44), 248 (38), 145 (100), 77 (92).

Anal. Calcd for $C_{18}H_{14}ClN_5O_2$: C, 58.78; H, 3.84; N, 19.04. Found: C, 58.62; H, 3.78; N, 19.16.

5-Aryloxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones (4)
To the solution of **2** prepared above in MeCN (15 mL) was added substituted phenol (2 mmol) and solid K_2CO_3 (0.04 g, 0.3 mmol). The mixture was stirred for 6–10 h at 40–50 °C and filtered, the filtrate was condensed and the residue was recrystallized (CH_2Cl_2–petroleum ether) to give 5-aryloxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-ones **4**.

3,6-Dihydro-3,6-diphenyl-5-(4-methoxyphenoxy)-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4q)
White crystals; mp 235–236 °C.

IR (KBr): 1752 (C=O), 1559, 1346, 1243 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.83 (s, 3 H), 6.89–7.98 (m, 14 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 55.66, 114.34 (2), 122.15 (2), 127.58 (2), 128.14, 128.26 (2), 129.26 (2), 129.43 (2), 129.66 (2), 134.16, 135.81, 144.94, 146.53, 155.35, 156.92, 157.73.

MS: *m*/*z* (%) = 411 (2) [M$^+$], 383 (1), 204 (3), 128 (12), 76 (100).

Anal. Calcd for $C_{23}H_{17}N_5O_3$: C, 67.15; H, 4.16; N, 17.02. Found: C, 67.34; H, 4.07; N, 17.15.

3,6-Dihydro-3,6-diphenyl-5-(4-methylphenoxy)-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4r)
White crystals; mp 209–211 °C.

IR (KBr): 1737 (C=O), 1549, 1348, 1249 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.38 (s, 3 H), 7.02–7.96 (m, 14 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.84, 120.67 (2), 120.91 (2), 128.14, 128.24 (2), 128.39, 129.24 (2), 129.41, 129.65 (2), 129.87 (2), 134.16, 135.81, 136.26, 146.52, 149.28, 155.35, 156.72.

MS: *m*/*z* (%) = 395 (2) [M$^+$], 367 (2), 204 (8), 128 (14), 76 (100).

Anal. Calcd for $C_{23}H_{17}N_5O_2$: C, 69.86; H, 4.33; N, 17.71. Found: C, 69.61; H, 4.16; N, 17.84.

3-(4-Chlorophenyl)-3,6-dihydro-5-(4-methoxyphenoxy)-6-(3-methylphenyl)-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4s)
White crystals; mp 200–201 °C.

IR (KBr): 1734 (C=O), 1560, 1505, 1350 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.45 (s, 3 H), 3.84 (s, 3 H), 6.91–7.95 (m, 12 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.32, 55.67, 114.33 (2), 121.64 (2), 122.16 (2), 124.99, 127.54, 128.56, 129.38 (4), 130.31, 133.90, 134.31, 139.76, 144.88, 146.49, 155.22, 157.20, 157.76.

MS: *m*/*z* (%) = 461/459 (17/52) [M$^+$], 430 (23), 396 (15), 314 (100), 152 (66).

Anal. Calcd for $C_{24}H_{18}ClN_5O_3$: C, 62.68; H, 3.95; N, 15.23. Found: C, 62.72; H, 3.91; N, 15.35.

3-(4-Chlorophenyl)-3,6-dihydro-5-(4-methylphenoxy)-6-(3-methylphenyl)-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4t)
White crystals; mp 210–211 °C.

IR (KBr): 1753 (C=O), 1550, 1507, 1352 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.40 (s, 3 H), 3.45 (s, 3 H), 7.01–7.95 (m, 12 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.88, 21.34, 120.96 (2), 121.65 (2), 125.01, 127.60, 128.58, 129.40 (2), 129.45 (2), 129.90 (2), 130.34, 133.91, 134.37, 136.38, 139.78, 146.51, 149.26, 155.26, 157.04.

MS: *m*/*z* (%) = 443 (5) [M^+], 415 (2), 338 (2), 110 (18), 89 (100).

Anal. Calcd for $C_{24}H_{18}ClN_5O_2$: C, 64.94; H, 4.09; N, 15.78. Found: C, 64.87; H, 4.15; N, 15.79.

3-(4-Chlorophenyl)-3,6-dihydro-6-(3-methylphenyl)-5-phenoxy-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4u)
White crystals; mp 228–230 °C.

IR (KBr): 1754 (C=O), 1551, 1511, 1355 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.46 (s, 3 H), 7.13–7.93 (m, 13 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.33, 121.39 (2), 121.58 (2), 125.00, 126.65, 127.57, 128.57, 129.34 (2), 129.49 (4), 130.36, 133.90, 134.28, 139.80, 146.40, 151.42, 155.20, 156.97.

MS: *m*/*z* (%) = 431/429 (2/6) [M^+], 401 (1), 323 (3), 110 (26), 76 (100).

Anal. Calcd for $C_{23}H_{16}ClN_5O_2$: C, 64.27; H, 3.75; N, 16.29. Found: C, 64.03; H, 3.58; N, 16.37.

5-(4-Chlorophenoxy)-3-(4-chlorophenyl)-3,6-dihydro-6-phenyl-7*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-one (4v)
White crystals; mp 248–249 °C.

IR (KBr): 1741 (C=O), 1559, 1350, 1082 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.10–7.59 (m, 11 H), 7.88 (d, *J* = 9.2 Hz, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 121.76 (2), 122.81 (2), 127.65, 128.06 (2), 129.51 (3), 129.58 (2), 129.76 (2), 132.16, 133.83, 134.21 (2), 146.24, 149.76, 154.99, 156.54.

MS: *m*/*z* (%) = 451/449 (4/6) [M^+], 421 (5), 386 (7), 136 (36), 110 (100).

Anal. Calcd for $C_{22}H_{13}Cl_2N_5O_2$: C, 58.68; H, 2.91; N, 15.55. Found: C, 58.55; H, 2.96; N, 15.49.

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