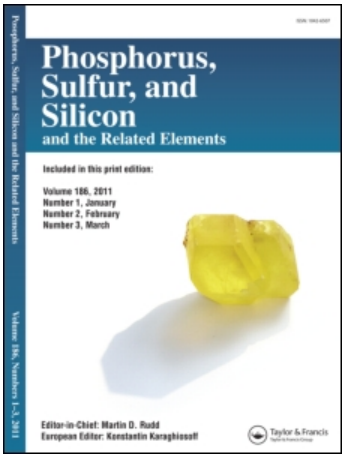

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Synthesis of Novel Derivatives of 5-(4,6-Dimethyl-2-Pyrimidinylsulfanyl)methyl-1,2,4-triazole-3-thione

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SYNTHESIS OF NOVEL DERIVATIVES OF 5-(4,6-DIMETHYL-2-PYRIMIDINYLSULFANYL)METHYL-1,2,4-TRIAZOLE-3-THIONE

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*Alkylation of 5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole-3-thione (**2**) with various alkyl halides, 4-chlorophenacyl bromide, chloroacetic acid, and α-chloroacetanilide afforded S-substituted 1,2,4-triazoles (**3–11**). 3-Carboxymethylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole (**9**), in the presence of acetic anhydride, was cyclized to 6-(4,6-dimethyl-2-pyrimidinylsulfanyl)methylthiazolo[3,2-*b*][1,2,4]triazol-3(2H)-one (**12**). The later condensed with aromatic aldehydes to give 6-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-6-[(1-aryl)methylidene]thiazolo[3,2-*b*][1,2,4]triazol-3(2H)-ones (**13**, **14**) and under treatment with aniline underwent ring-disclosure reaction to yield 3-(phenylcarbamoyl)methylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole (**11**).*

Keywords: Alkylation; cyclization; substituted 1,2,4-triazole-3-thiones; thiazolo[3,2-*b*]triazolone

A number of bioactive molecules contain functionalized azole and azine heterocycles. A 1,2,4-triazole moiety is a key component in the structure of potential anticancer,[1] antimigraine[2–4] agents. 1,2,4-Triazole derivatives have been reported to exhibit antimicrobial,[5–7] antitubercular,[8] serotonergic[9] activity, and plant protecting properties.[7,10,11] Triazole ring formation reactions, as well as the rich chemistry of fused or pendant 1,2,4-triazoles, are the subject of research in previous and recent reports.[12–17] Our earlier studies involved synthesis of heterocyclic compounds containing in their structures both the pyrimidine and 1,2,4-triazole fragments.[18–20] In this connection and in continuation of our

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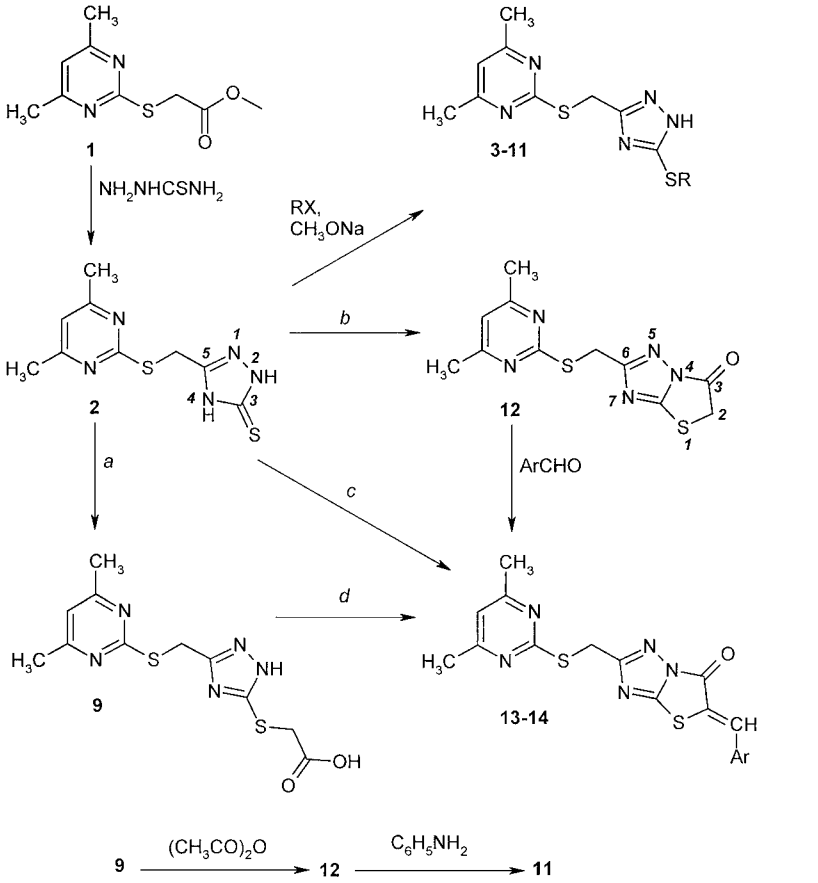
interest in the synthesis of chemically and biologically important heterocycles, we now report on 5-(pyrimidinylsulfanyl)methyl substituted 1,2,4-triazoles.

RESULTS AND DISCUSSION

Triazole **2** was prepared by the condensation reaction of ester **1** with thiosemicarbazide in the presence of sodium methoxide. While optimizing this reaction, we found that an excess of thiosemicarbazide and long reaction times were necessary for high yields of desired product **2**. It was observed that work-up of the reaction mixture with acetic acid instead of hydrochloric acid as well as using low temperatures (~5°C) with the reaction mixture was preferable.

The alkylation of triazole **2** with various alkylating agents was studied, and 3-alkyl substituted derivatives **3–11** were obtained. These reactions were carried out in methanol/sodium methoxide solution affording yields of compounds **3–11** from moderate to high (57–94%). Noteworthy was the use of triethylamine as a base instead of sodium methoxide, which did not influence reaction time nor yield of compounds. The yields varied depending on alkylating agent used. Formation of alkyl derivatives **3–6** was achieved in 1–2 h. Alkylation of **2** with 4-chlorophenacyl bromide was complete within 0.5 h in high yield of **8** (91%), while the reaction of **2** with α-chloroacetanilide proceeded in 8 h to give a poor yield of compound **11** (37%). Acid **9** was synthesized analogously in moderate yield (66%). Acid **9** also was synthesized by a more efficient and simple method. Thus, triazole **2** reacted with chloroacetic acid in glacial acetic acid at reflux in the presence of anhydrous sodium acetate to give an excellent yield (94%) of acid **9**. The IR spectra of compounds **3–11** display intensive absorption bands at 1260–1268 cm^{-1},characteristic for S-alkylated 1,2,4-triazoles,[21] and the absorption for N—C=S in the region of 1337 cm^{-1}, characteristic for 1,2,4-triazole-2-thione, was absent. Treatment of acid **9** with acetic anhydride at reflux induced cyclisation to occur and yielded thiazolo[3,2-*b*]triazolone **12**. Moreover, the same compound **12** was obtained from the triazole **2** in a one-pot, four-component cycloalkylation reaction, i.e., on heating of the mixture of triazole **2**, chloroacetic acid, acetic anhydride, and anhydrous sodium acetate in acetic acid. Cyclisation of acid **9** by the action of acetic anhydride may occur either at N-2 or at the N-4 atom. The N-2 atom is more likely involved in the cyclisation reaction because of its greater basicity.[22,23] The ^1H NMR spectra of compounds **9** and **12** support the structures and this type of reaction. If cyclization would take place at N-4 atom, one would expect influence by the carbonyl group on neighbouring protons



Reagents: *a* : $ClCH_2CO_2H$, CH_3CO_2Na, CH_3CO_2H

b : $ClCH_2CO_2H$, CH_3CO_2Na, $(CH_3CO)_2O$, CH_3CO_2H

c : $ClCH_2CO_2H$, CH_3CO_2Na, $(CH_3CO)_2O$, ArCHO, CH_3CO_2H

d : $(CH_3CO)_2O$, ArCHO, CH_3CO_2H

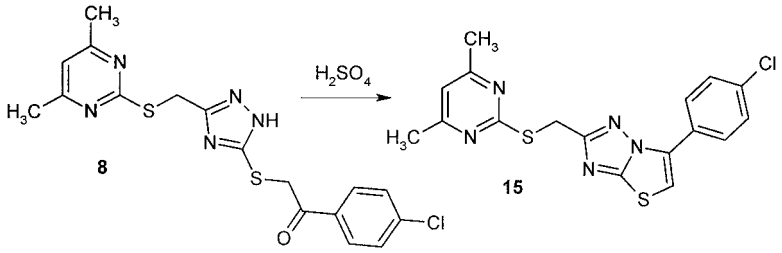
X = Cl, Br; R = **3** - *n*-C_3H_7 , **4** - *n*-C_4H_9, **5** - *n*-$C_{10}H_{21}$, **6** - $CH_2CH{=}CH_2$, **7** - $CH_2C_6H_5$, **8** - $CH_2COC_6H_4$-4-Cl, **9** - CH_2CO_2H, **10** - $CH_2CO_2C_2H_5$, **11** - $CH_2CONHC_6H_5$;

Ar = **13** - C_6H_5, **14** - 4-CH_3O-C_6H_4

SCHEME 1

to be markedly shifted downfield.[23,24] Shifts of the CH_2S group protons of acid **9** and the corresponding shift of the CH_2S protons of cyclic compound **12** have almost the same values. The IR spectrum of compound **12** displayed an intense absorption band at 1769 cm^{-1}. Absorption in this

region is characteristic for ring-fused thiazolotriazolones.[25] The methylene groups (C-2) of compound **12** condensed with aromatic aldehydes to give compounds **13**, **14**. The latter also were prepared by the reaction of acid **9** and aromatic aldehyde in the presence of acetic anhydride or by direct reaction of the mixture of triazole **2**, chloroacetic acid, acetic anhydride, an aromatic aldehyde, and sodium acetate in acetic acid. In the ^{1}H NMR spectra of compounds **13**, **14**, characteristic chemical shifts of CH_2S protons are observed in the same region (4.59–4.61 ppm) as those for compound **12**. Moreover, compounds **13**, **14** display signals characteristic of methine protons (8.19–8.26 ppm) and signals of aromatic protons (7.21–7.90 ppm). In the IR spectra, due to conjugation of the C=O with double bonds, the absorption bands for the C=O group in compounds **13**, **14** are observed at lower frequencies (23–35 cm^{-1}) compared with that of compound **12**. Thiazolotriazolone ring of **12** under treatment with an excess of aniline was easily opened to give anilide **11**. Thus, the said conversion is expedient for the synthesis of compound **9** since the alkylation reaction of triazole **2** with α-chloroacetanilide to obtain compound **11** was not so successful.



SCHEME 2

The action of concentrated sulfuric acid on compound **8** at 0°C induced the thiazolotriazolone ring closure with formation of compound **15**. The shift of CH_2S protons of **15** is in the same region as those of thiazolotriazoles **12–14**. Also a characteristic signal of the vinyl proton occured at 7.91 ppm in the ^{1}H NMR spectra of **15**.

Compounds were preliminary tested for their anti-inflammatory activity. Several of compounds, i.e., **2**, **4**, **9**, exhibited slight anti-inflammatory activity induced in rats by bentonite and carrageenin.

EXPERIMENTAL

Melting points were determined in open capillaries and are uncorrected. The IR spectra were measured on a Spectrum BX FT-IR (Perkin-Elmer) in Nujol, ^{1}H-NMR spectra were recorded on a BS-587A (80 MHz,

Tesla) in DMSO-d_6 with TMS as an internal standard. Chemical shifts (δ) are reported in ppm and coupling constants (J) are given in Hz. The reactions were monitored by TLC on silica gel coated Al plates (KAVALIER). Elemental analyses were performed at the Microanalysis Laboratory of the Department of Organic Chemistry of Vilnius University. Methyl (4,6-dimethyl-2-pyrimidinylsulfanylmethyl)acetate (**1**) was synthesised according literature.[26]

5-(4,6-Dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole-3-thione (2)

A mixture of ester **1** (10 mmol, 2.12 g), thiosemicarbazide (10 mmol, 0.91 g), and sodium methoxide (10 mmol, 0.23 g of sodium dissolved in 15 ml CH_3OH) was refluxed in CH_3OH (30 ml) for 20 h. The solvent was removed in vacuo, and the residue was dissolved in H_2O (50 ml), acidified carefully with acetic acid (at 0–5°C) to pH 6, filtered, and recrystallized from isopropanol. Yield 1.67 g (66%), m.p. 216–217°C. Anal. calcd. for $C_9H_{11}N_5S_2$ (253.35): C, 42.67; H, 4.38; N, 27.64. Found: C, 42.82; H, 4.49; N, 27.88. ^{1}H NMR: 2.37 (s, 6H, 2 CH_3), 4.35 (s, 2H, CH_2S), 6.99 (s, 1H, CH), 13.26 (s, 1H, NH). IR (cm^{-1}): 3086 (NH), 1572, 1532 (C=C, C=N), 1337 (N–C=S).

3-Alkyl Substituted 5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazoles (3–11) *(General Procedure)*

To a stirred solution of triazole **2** (5 mmol, 1.27 g) and sodium methoxide (5 mmol, 0.115 g of sodium dissolved in 10 ml CH_3OH) in CH_3OH (20 ml) was added dropwise a solution of alkyl halide (5 mmol) in CH_3OH (10 ml). The reaction mixture was refluxed for 1–2 h and filtered off. The filtrate was concentrated in vacuo, and the residue was filtered and recrystallized from appropriate solvent.

5-(4,6-Dimethyl-2-pyrimidinylsulfanyl)methyl-3-propylsulfanyl-1,2,4-triazole (3)

Yield 52%, m.p. 57–58°C (from hexane). Anal. calcd. for $C_{12}H_{17}N_5S_2$ (295.43): C, 48.81; H, 5.76; N, 23.73. Found: C, 49.06; H, 5.53; N, 23.81. ^{1}H NMR: 0.97 (t, $J = 4$ Hz, 3H, CH_3), 1.62 (m, 2H, CH_2), 2.35 (s, 6H, 2 CH_3), 3.03 (t, $J = 4$ Hz, 2H, SCH_2-3), 4.40 (s, 2H, CH_2S-5), 6.98 (s, 1H, CH), 13.79 (s, 1H, NH). IR (cm^{-1}): 3115 (NH), 1583, 1533 (C=C, C=N), 1268 (S-alkyl 1,2,4-triazoles).

3-Butylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl) methyl-1,2,4-triazole (4)

Yield 73%, m.p. 70–71°C (from hexane). Anal. calcd. for $C_{13}H_{19}N_5S_2$ (309.46): C, 50.46; H, 6.19; N, 22.63. Found: C, 50.38; H, 6.36; N, 22.84. ^{1}H NMR: 1.29 (t, $J = 6$ Hz, 3H, CH_3), 1.89 (m, 4H, 2 CH_2), 2.38 (s, 6H, 2 CH_3), 3.07 (t, $J = 6$ Hz, 2H, SCH_2-3), 4.45 (s, 2H, CH_2S-5), 6.98 (s, 1H, CH), 13.78 (s, 1H, NH). IR (cm^{-1}): 3148 (NH), 1584, 1533 (C=C, C=N), 1266 (S-alkyl 1,2,4-triazoles).

3-Decylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl) methyl-1,2,4-triazole (5)

Yield 49%, m.p. 36–37°C (from hexane). Anal. calcd. for $C_{19}H_{31}N_5S_2$ (393.62): C, 58.02; H, 7.89; N, 17.81. Found: C, 58.15; H, 7.76; N, 17.89. ^{1}H NMR: 0.86 (t, $J = 4$ Hz, 3H, CH_3), 1.25 (m, 16H, 8 CH_2), 2.37 (s, 6H, 2 CH_3), 3.07 (t, $J = 4$ Hz, 2H, SCH_2-3), 4.45 (s, 2H, CH_2S-5), 6.99 (s, 1H, CH), 13.20 (s, 1H, NH). IR (cm^{-1}): 3156 (NH), 1586, 1537 (C=C, C=N), 1267 (S-alkyl 1,2,4-triazoles).

3-Allylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl) methyl-1,2,4-triazole (6)

Yield 65%, m.p. 64–65°C (from hexane). Anal. calcd. for $C_{12}H_{15}N_5S_2$ (293.42): C, 49.15; H, 5.12; N, 23.89. Found: C, 49.22; H, 5.10; N, 23.70. ^{1}H NMR: 2.41 (s, 6H, 2 CH_3), 3.77 (d, $J = 4$ Hz, 2H, SCH_2-3), 4.49 (s, 2H, CH_2S-5), 5.15, 5.34 (2s, 2H, CH_2), 5.93 (m, 1H, CH), 7.03 (s, 1H, CH), 13.88 (s, 1H, NH). IR (cm^{-1}): 3082 (NH), 1581, 1532 (C=C, C=N), 1265 (S-alkyl 1,2,4-triazoles).

3-Benzylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl) methyl-1,2,4-triazole (7)

Yield 85%, m.p. 91–93°C (from cyclohexane). Anal. calcd. for $C_{16}H_{17}N_5S_2$ (343.48): C, 55.98; H, 4.96; N, 20.41. Found: C, 55.80; H, 5.02; N, 20.44. ^{1}H NMR: 2.37 (s, 6H, 2 CH_3), 4.34 (s, 2H, SCH_2-3), 4.48 (s, 2H, CH_2S-5), 7.00 (s, 1H, CH), 7.30 (m, 5H, C_6H_5), 13.86 (s, broad, 1H, NH). IR (cm^{-1}): 3105 (NH), 1582, 1532 (C=C, C=N), 1260 (S-alkyl 1,2,4-triazoles).

3-[(4-Chlorophenyl)carbonylmethylsulfanyl]-5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole (8)

Yield 91%, m.p. 104–105°C (from H_2O + CH_3OH). Anal. calcd. for $C_{17}H_{16}ClN_5OS_2$ (389.93): C, 50.31; H, 3.95; N, 17.26. Found: C, 49.96;

H, 3.95; N, 17.33. ^{1}H NMR: 2.35 (s, 6H, 2 CH_3), 4.43 (s, 2H, CH_2S-5), 4.79 (s, 2H, SCH_2-3), 6.98 (s, 1H, CH), 7.61 (d, $J = 6$ Hz, 2H, aromatic), 8.04 (d, $J = 6$ Hz, 2H, aromatic). IR (cm^{-1}): 3054 (NH), 1683 (CO), 1587, 1532 (C=C, C=N), 1268 (S-alkyl 1,2,4-triazoles).

3-Carboxymethylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole (9)

Method A

A mixture of triazole **2** (3.8 mmol, 0.95 g), chloroacetic acid (3.8 mmol, 0.36 g), and sodium methoxide (7.6 mmol, 0.175 g of sodium dissolved in 10 ml CH_3OH) in CH_3OH (30 ml) was heated at reflux for 2 h. After the solvent was evaporated, the residue was dissolved in ice-cold water and acidified with acetic acid. The solid formed was filtered off and recrystallized from H_2O. Yield 0.77 g (66%).

Method B

A mixture of triazole **2** (3.8 mmol, 0.95 g), chloroacetic acid (3.8 mmol, 0.36 g), and sodium acetate (0.49 g, 6 mmol) in acetic acid (30 ml) was heated at reflux for 2 h. Then the solution was evaporated to dryness, and the residue was recrystallized from H_2O. Yield 0.88 g (75%), m.p. 84–85°C. Anal. calcd. for $C_{11}H_{13}N_5O_2S_2$ (311.39): C, 42.43; H, 4.21; N, 22.49. Found: C, 42.25; H, 4.27; N, 22.27. ^{1}H NMR: 2.40 (s, 6H, 2 CH_3), 3.93 (s, 2H, SCH_2-3), 4.46 (s, 2H, CH_2S-5), 6.96 (s, 1H, CH), 14.2 (s, broad, 1H, NH). IR (cm^{-1}): 3135 (NH); 1694, (CO), 1589, 1537 (C=C, C=N), 1269 (S-alkyl 1,2,4-triazoles).

3-Ethoxycarbonylmethylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole (10)

Yield 74%, m.p. 95–96°C. Anal. calcd. for $C_{12}H_{15}N_5O_2S_2$ (325.42): C, 44.31; H, 4.62; N, 21.54. Found: C, 44.58; H, 4.56; N, 21.47. ^{1}H NMR: 1.16 (t, $J = 6$ Hz, 3H, CH_3), 2.36 (s, 6H, 2 CH_3), 3.97 (s, 2H, SCH_2-3), 4.05 (q, $J = 6$ Hz, 2H, OCH_2), 4.45 (s, 2H, CH_2S-5), 6.99 (s, 1H, CH), 13.92 (s, broad, 1H, NH). IR (cm^{-1}): 3098 (NH), 1726 (CO), 1590, 1530 (C=C, C=N), 1265 (S-alkyl 1,2,4-triazoles).

3-(Phenylcarbamoyl)methylsulfanyl-5-(4,6-dimethyl-2-pyrimidinylsulfanyl)methyl-1,2,4-triazole (11)

Method A

As described in *General procedure* for compounds **3–11**. Reaction time 8 h. Yield, 37%.

Method B

A mixture of compound **12** (1.3 mmol, 0.38 g) and aniline (5.2 mmol, 4.84 g, 4.74 ml) was refluxed in *n*-propanol (8 ml) for 2 h. After cooling, the product was filtered off and recrystallized from isopropanol. Yield 0.31 g (65%), m.p. 172–173°C. Anal. calcd. for $C_{17}H_{18}N_6OS_2$ (386.5): C, 52.83; H, 4.69; N, 21.74. Found: C, 53.10; H, 4.67; N, 21.81. ^{1}H NMR: 2.37 (s, 6H, 2 CH_3), 4.07 (s, 2H, SCH_2-3), 4.48 (s, 2H, CH_2S-5), 6.80 (s, 1H, CH), 7.30 (m, 5H, C_6H_5), 13.90 (s, broad, 1H, NH). IR (cm^{-1}): 3292, 3189 (NH), 1666 (CO), 1585, 1535 (C=C, C=N), 1264 (S-alkyl 1,2,4-triazoles).

6-(4,6-Dimethyl-2-pyrimidinylsulfanyl) methylthiazolo[3,2-*b*][1,2,4]triazol-3(2*H*)-one (12)

Method A

An acid **9** (1.6 mmol, 0.5 g) was refluxed in acetic anhydride (7 ml) for 2 h, and then the reaction mixture was cooled and poured into ice-water. The solid was filtered off, dried and recrystallized from benzene. Yield 0.38 g (81%), m.p. 143–145°C. Anal. calcd. for $C_{11}H_{11}N_5OS_2$ (293.37): C, 42.43; H, 4.21; N, 22.49. Found: C, 41.80; H, 4.47; N, 22.27. ^{1}H NMR: 2.36 (s, 6H, 2 CH_3), 4.64 (s, 2H, CH_2S-6), 4.52 (s, 2H, CH_2-2), 7.00 (s, 1H, CH). IR (cm^{-1}): 1769 (CO), 1576, 1508 (C=C, C=N), 1265 (S-alkyl 1,2,4-triazoles).

Method B

A mixture of triazole **2** (5 mmol, 1.27 g), chloroacetic acid (8 mmol 0.76 g), sodium acetate (12 mmol, 0.98 g) in acetic acid (10 ml)-acetic anhydride (15 ml) solution was refluxed for 2 h and worked as above. Yield 1.12 g (77%).

6-(4,6-Dimethyl-2-pyrimidinylsulfanyl)methyl-2-[(1-aryl) methylidene]thiazolo[3,2-*b*] [1,2,4]triazol-3(2*H*)-ones (13–14)

Method A

A mixture of triazole **2** (5 mmol, 1.27 g), chloroacetic acid (8 mmol, 0.76 g), sodium acetate (12 mmol, 0.98 g) and an aromatic aldehyde (8 mmol) in acetic acid ((10 ml)—acetic) anhydride (15 ml) solution was refluxed for 2 h. When cooled, the precipitate was filtered off, washed with water and ethanol, and recrystallized from *n*-butanol.

Method B

A mixture of acid **9** (4 mmol, 1.25 g) and an aromatic aldehyde (4 mmol) in acetic acid (10 ml)-acetic anhydride (7 ml) solution was heated at 90°C for 2 h and decomposed as above.

Method C

A mixture of compound **12** (4 mmol, 1.17 g) and an aromatic aldehyde (4 mmol) in acetic acid (10 ml) was heated at 95–100°C for 1 h and decomposed as above.

6-(4,6-Dimethyl-2-pyrimidinylsulfanyl)methyl-2-[(phenyl) methylidene]thiazolo[3,2-*b*][1,2,4]triazol-3(2*H*)-one (13)

Yield 78%, m.p. 180–182°C. Anal. calcd. for $C_{18}H_{15}N_5OS_2$ (381.48): C, 56.67; H, 3.96; N, 18.36. Found: C, 56.78; H, 4.27; N, 18.31. ^{1}H NMR: 2.39 (s, 6H, 2 CH_3), 4.61 (s, 2H, CH_2S-6), 7.00 (s, 1H, CH pyrimidine), 7.70 (m, 5H, C_6H_5), 8.26 (s, 1H, CH). IR (cm^{-1}): 1746 (CO), 1588, 1520 (C=C, C=N), 1268 (S-alkyl 1,2,4-triazoles).

6-(4,6-Dimethyl-2-pyrimidinylsulfanyl)methyl-2-[(4-methoxyphenyl)methylidene]thiazolo[3,2-*b*][1,2,4] triazol-3(2*H*)-one (14)

Yield 75%, m.p. 202–204°C. Anal. calcd. for $C_{19}H_{17}N_5O_2S_2$ (411.51): C, 55.46; H, 4.16; N, 17.02. Found: C, 55.66; H, 4.31; N, 17.27. ^{1}H NMR: 2.43 (s, 6H, 2 CH_3), 3.93 (s, 3H, OCH_3), 4.59 (s, 2H, CH_2S-6), 7.00 (s, 1H, CH pyrimidine), 7.11 (d, $J = 6$ Hz 2H, aromatic), 7.69 (d, $J = 6$ Hz 2H, aromatic), 8.19 (s, 1H, CH). IR (cm^{-1}): 1734 (CO), 1585, 1513 (C=C, C=N), 1267 (S-alkyl 1,2,4-triazoles).

3-(4-Chlorophenyl)-6-(4,6-dimethyl-2-pyrimidinylsulfanyl)methylthiazolo[3,2-*b*][1,2,4] triazole (15)

Compound **8** (1.48 mmol, 0.6 g) was stirred in conc. H_2SO_4 (4 ml) at 0°C for 0.5 h. Then the mixture was diluted with ice-cold water (15 ml) and neutralized with 15% KOH solution. The precipitate was filtered off, washed with water and methanol, and recrystallized from benzene. Yield 75%, m.p. 188–190°C. Anal. calcd. for $C_{17}H_{14}ClN_5S_2$ (387.92): C, 52.64; H, 3.64; N, 18.05. Found: C, 52.96; H, 3.72; N, 18.19. ^{1}H NMR: 2.38 (s, 6H, 2 CH_3), 4.65 (s, 2H, CH_2S-6), 6.96 (s, 1H, CH pyrimidine), 7.61 (d, $J = 6$ Hz 2H, aromatic), 7.91 (s, 1H, CH), 8.23 (d, $J = 6$ Hz 2H, aromatic). IR (cm^{-1}): 1584, 1534 (C=C, C=N), 1267 (S-alkyl 1,2,4-triazoles).

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