

Convenient synthesis of new pyrimido[4,5-*e*][1,3,4]thiadiazine derivatives

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Characteristics of compounds **3c-e** and **4c-f**.

7-Chloro-5-methyl-1-phenyl-3-(propylsulfanyl)-1*H*-pyrimido[4,5-*e*][1,3,4]thiadiazine (3c)

This compound was obtained as a yellow powder in 45% yield, mp 81-82°C, IR (KBr disk): ν , 850 cm^{-1} , 1650 cm^{-1} , 2900 cm^{-1} , 2950 cm^{-1} ; $^1\text{HNMR}$: (CDCl_3) δ , 1.09 (t, 3H, CH_3 , J 7.3 Hz), 1.7 (sextet, 2H, CH_2), 2.35 (s, 3H, 8- CH_3), 3.06 (t, 2H, S- CH_2 , J 7.3 Hz), 7.2-7.6 (multiplet, 5H), m/z, 352, 351, 350, 349, 277, 275, 74; *Anal.* Calc. for $\text{C}_{15}\text{H}_{15}\text{ClN}_4\text{S}_2$ (%): C, 51.34; H, 4.31; N, 15.97; S, 18.28. Found (%): C, 51.42; H, 4.35; N, 15.81; S, 18.13.

3-(Butylsulfanyl)-7-chloro-5-methyl-1-phenyl-1*H*-pyrimido[4,5-*e*][1,3,4]thiadiazine (3d)

This compound was obtained as a yellow powder in 40% yield, mp 56-58°C, IR (KBr disk): ν , 830 cm^{-1} , 1600 cm^{-1} , 2900 cm^{-1} , 2960 cm^{-1} ; $^1\text{HNMR}$: (CDCl_3) δ , 0.95 (t, 3H, CH_3 , J 7.1 Hz), 1.3-1.8 (multiplet, 4H, 2 CH_2), 2.35 (s, 3H, 8- CH_3), 3.1 (t, 2H, S- CH_2 , J 7.2 Hz), 7.2-7.6 (multiplet, 5H) m/z, 366, 365, 364, 363, 277, 275, 88; *Anal.* Calc. for $\text{C}_{16}\text{H}_{17}\text{ClN}_4\text{S}_2$ (%): C, 52.66; H, 4.70; N, 15.35; S, 17.57. Found (%): C, 52.57; H, 4.75; N, 15.40; S, 17.41.

3-(Benzylsulfanyl)-7-chloro-5-methyl-1-phenyl-1*H*-pyrimido[4,5-*e*][1,3,4]thiadiazine (3e)

This compound was obtained as a yellow powder in 70% yield, mp 121-123°C, IR (KBr disk): ν , 880 cm^{-1} , 1550 cm^{-1} , 2900 cm^{-1} , 2940 cm^{-1} ; $^1\text{HNMR}$: (CDCl_3) δ , 2.33 (s, 3H, 8- CH_3), 4.29 (s, 2H, S- CH_2), 7.2-7.5 (multiplet, 10H); m/z, 400, 399, 398, 397, 277, 275, 122; *Anal.* Calc. for $\text{C}_{19}\text{H}_{15}\text{ClN}_4\text{S}_2$ (%): C, 57.20; H, 3.79; N, 14.04; S, 16.08. Found (%): C, 57.32; H, 3.75; N, 14.18; S, 15.95.

4-[5-Methyl-1-phenyl-3-(propylsulfanyl)-1H-pyrimido[4,5-*e*][1,3,4]thiadiazin-7-yl]morpholine (4c)

This compound was obtained as a green powder in 80% yield, mp 89-91°C, IR (KBr disk): ν , 1580 cm^{-1} , 2900 cm^{-1} , 2940 cm^{-1} ; $^1\text{H NMR}$: (CDCl_3) δ , 1 (t, 3H, CH_3 , 6.9 Hz), 1.7 (sextet, 2H, CH_2), 2.26 (s, 3H, 8- CH_3), 3.05 (t, 2H, S- CH_2 , 7.1 Hz), 3.57 (m, 8H, CH_2 -(O&N)), 7.2-7.6 (multiplet, 5H); m/z , 401; *Anal.* Calc. for $\text{C}_{19}\text{H}_{23}\text{N}_5\text{OS}_2$ (%): C, 56.83; H, 5.77; N, 17.44; S, 15.97. Found (%): C, 56.94; H, 5.80; N, 17.52; S, 15.81.

5-Methyl-1-phenyl-3-(propylsulfanyl)-7-tetrahydro-1H-1-pyrrolyl-1H-pyrimido[4,5-*e*][1,3,4]thiadiazine (4d)

This compound was obtained as a green powder in 65% yield, mp 98°C IR (KBr disk): ν , 1640 cm^{-1} , 2900 cm^{-1} , 2960 cm^{-1} ; $^1\text{H NMR}$: (CDCl_3) δ , 1 (t, 3H, CH_3 , 7.5 Hz), 1.7 (sextet, 2H, CH_2), 2.26 (m, 7H, 8- CH_3 & 2 ((CH_2)- CH_2N)), 3.05 (t, 2H, S- CH_2 , 7.3 Hz), 3.58 (br, 4H, 2(CH_2N)), 7.2-7.6 (multiplet, 5H); m/z , 385; *Anal.* Calc. for $\text{C}_{19}\text{H}_{23}\text{N}_5\text{S}_2$ (%): C, 59.19; H, 6.01; N, 18.16; S, 16.63. Found (%): C, 59.10; H, 5.92; N, 18.28; S, 16.49.

4-[3-(Benzylsulfanyl)-5-methyl-1-phenyl-1H-pyrimido[4,5-*e*][1,3,4]thiadiazin-7-yl]morpholine (4e)

This compound was obtained as a green powder in 85% yield, mp 139-141°C, IR (KBr disk): ν , 1580 cm^{-1} , 2900 cm^{-1} , 2970 cm^{-1} ; $^1\text{H NMR}$: (CDCl_3) δ , 2.24 (s, 3H, 8- CH_3), 3.50 (m, 8H, CH_2 -(O&N)), 4.30 (s, 2H, S- CH_2), 7.2-7.6 (multiplet, 10H); m/z , 449; *Anal.* Calc. for $\text{C}_{23}\text{H}_{23}\text{N}_5\text{OS}_2$ (%): C, 61.44; H, 5.16; N, 15.58; S, 14.26. Found (%): C, 61.56; H, 5.24; N, 15.52; S, 14.11.

3-(Benzylsulfanyl)-5-methyl-1-phenyl-7-tetrahydro-1H-1-pyrrolyl-1H-pyrimido[4,5-*e*][1,3,4]thiadiazine (4f)

This compound was obtained as a green powder in 75% yield, mp 128-130°C, IR (KBr disk): ν , 1640 cm^{-1} , 2900 cm^{-1} , 2950 cm^{-1} ; $^1\text{H NMR}$: (CDCl_3) δ , 1.93 (t, 4H, 2 ((CH_2)- CH_2N), 6.1 Hz), 2.26 (s, 3H, 8- CH_3), 3.30 (br, 4H, 2(CH_2N)), 4.32 (s, 2H, S- CH_2), 7.2-7.6 (multiplet, 10H); m/z , 433; *Anal.* Calc. for $\text{C}_{23}\text{H}_{23}\text{N}_5\text{S}_2$ (%): C, 63.71; H, 5.35; N, 16.15; S, 14.79. Found (%): C, 63.56; H, 5.42; N, 16.20; S, 14.63.