Supplementary Material

Synthesis of pyrimido[2,1-*b*][1,3]benzothiazoles and [1,3]benzothiazolo [3,2-*a*]quinazolines *via* one-pot three-component reactions from 2-aminobenzothiazole, arylglyoxals and 1,3-dicarbonyl compounds

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Experimental Section

General. All chemicals were purchased from Aldrich and Merck with high-grade quality, and used without any purification. All melting points were obtained by Barnstead Electrothermal 9200 apparatus and are uncorrected. The reactions were monitored by TLC and all yields refer to isolated products. NMR spectra were obtained on a Varian 500 MHz spectrometer (^{1}H NMR at 500 MHz, ^{13}C NMR at 125 MHz) in DMSO using TMS as an internal standard. Infrared spectra were recorded on a Bruker FT-IR Equinax-55 spectrophotometer in KBr with absorption in cm^{-1}. Elemental analyses were performed using a Carlo Erba EA 1108 instrument. All products were characterized by their spectral and physical data.

1.2. General procedure for the synthesis of compounds 4a-e

A mixture of arylglyoxal **1** (1.0 mmol), 2-aminobenzothiazole **2** (0.9 mmol), and Meldrum's acid **3** (1.0 mmol) was stirred in 5.0 mL of acetic acid under reflux conditions for 130-180 min. After completion of the reaction, determined by TLC, the solvent was removed under reduced pressure, and the viscous residue was purified by plate chromatography (20×20 cm) using n-hexane/EtOAc (2:1) as eluent to give the pure compounds **4a–e** (55–68%).

1.3. General procedure for the synthesis of compounds 6a-f

A mixture of arylglyoxal **1** (1.0 mmol), 2-aminobenzothiazole **2** (0.9 mmol), and dimedone **5** (1.0 mmol) was stirred in 5.0 mL of acetic acid under reflux conditions for 50-80 min. After completion of the reaction, determined by TLC, the solvent was removed under reduced pressure, and the resulting crude product was recrystallized from ethanol to give the pure compounds **6a–f** (70–85%).

1.4. General procedure for the synthesis of compounds 8a-i

A mixture of arylglyoxal **1** (1.0 mmol), 2-aminobenzothiazole **2** (0.9 mmol), and barbituric acid **7** (1.0 mmol) was stirred in 5.0 mL of acetic acid under reflux conditions for 15-40 min. After completion of the reaction, determined by TLC, the solvent was removed under reduced pressure, and the resulting crude product was recrystallized from ethanol to give the pure compounds 8a-i (80–95%).

2-(4-Methylbenzoyl)-4*H*-pyrimido[2,1-*b*][1,3]benzothiazol-4-one (**4a**)**.** Yellow oil. IR ν/cm^{-1} (KBr): 1676, 1603, 1495; ^{1}H NMR (500 MHz, DMSO): δ 2.46 (s, 3H, CH_3), 6.87 (s, 1H, CH), 7.32 (d, *J* 7.5 Hz, 2H, ArH), 7.55-7.61 (m, 2H, A-H), 7.75 (d, *J* 7.5 Hz, 1H, ArH), 7.94 (d, *J* 7.5 Hz, 2H, ArH), 9.16 (d, *J* 7.5 Hz, 1H, ArH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 21.8, 109.8, 120.3, 121.3, 121.9, 122.7, 124.6, 127.2, 127.6, 129.2, 130.7, 132.3, 132.4, 144.9, 161.0, 191.5 ppm. Anal. Calcd for $C_{18}H_{12}N_2O_2S$ (320.37): C, 67.48; H, 3.78; N, 8.74. Found: C, 67.31; H, 3.75; N, 8.79 %.

2-(4-Chlorobenzoyl)-4*H*-pyrimido[2,1-*b*][1,3]benzothiazol-4-one (**4b**)**.** Yellow oil. IR ν/cm^{-1} (KBr): 1682, 1583, 1494; ^{1}H NMR (500 MHz, DMSO): δ 6.93 (s, 1H, CH), 7.50 (d, *J* 7.5 Hz, 2H, ArH), 7.56-7.62 (m, 2H, ArH), 7.77 (d, *J* 7.5 Hz, 1H, ArH), 8.03 (d, *J* 7.5 Hz, 2H, ArH), 9.16 (d, *J* 7.5 Hz, 1H, ArH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 109.9, 109.9, 117.8, 120.3, 121.9, 123.2, 127.3, 127.7,

128.8, 132.0, 133.1, 133.3, 140.2, 179.1, 190.3 ppm. Anal. Calcd for $C_{17}H_9ClN_2O_2S$ (340.78): C, 59.92; H, 2.66; N, 8.22. Found: C, 60.07; H, 2.68; N, 8.19 %.

2-(4-Bromobenzoyl)-4*H*-pyrimido[2,1-*b*][1,3]benzothiazol-4-one (4c). Yellow oil. IR ν/cm^{-1} (KBr): 1669, 1582, 1493; ^{1}H NMR (500 MHz, DMSO): δ 6.93 (s, 1H, CH), 7.57-7.62 (m, 2H, ArH), 7.67 (d, *J* 7.5 Hz, 2H, ArH), 7.76 (d, *J* 7.5 Hz, 1H, ArH), 7.94 (d, *J* 7.5 Hz, 2H, ArH), 9.16 (d, *J* 7.5 Hz, 1H, ArH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 109.9, 110.6, 119.1, 120.3, 121.9, 124.7, 127.3, 128.0, 129.5, 131.8, 132.0, 133.0, 139.0, 179.4, 191.6 ppm. Anal. Calcd for $C_{17}H_9BrN_2O_2S$ (385.24): C, 53.00; H, 2.35; N, 7.27. Found: C, 53.11; H, 2.36; N, 7.24 %.

2-Benzoyl-4*H*-pyrimido[2,1-*b*][1,3]benzothiazol-4-one (**4d**). Yellow oil. IR ν/cm^{-1} (KBr): 1683, 1596, 1506; ^{1}H NMR (500 MHz, DMSO): δ 6.89 (s, 1H, CH), 7.53 (d, *J* 7.5 Hz, 2H, ArH), 7.56-7.60 (m, 2H, ArH), 7.65 (t, *J* 7.5 1H, Hz, ArH), 7.75 (d, *J* 7.5 Hz, 1H, ArH), 8.04 (d, *J* 7.5 Hz, 2H, ArH), 9.16 (d, *J* 7.5 Hz, 1H, ArH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 106.5, 109.9, 120.3, 121.9, 124.6, 127.2, 127.6, 128.4, 130.5, 130.8, 133.7, 135.0, 135.7, 156.8, 191.8 ppm.

2-(4-Fluorobenzoyl)-4*H*-pyrimido[2,1-*b*][1,3]benzothiazol-4-one (4e). Yellow oil. IR ν/cm^{-1} (KBr): 1617, 1594, 1509; ^{1}H NMR (500 MHz, DMSO): δ 6.92 (s, 1H, CH), 7.20 (d, *J* 7.5 Hz, 2H, ArH), 7.56-7.62 (m, 2H, ArH), 7.76 (d, *J* 7.5 Hz, 1H, ArH), 8.12 (d, *J* 7.5 Hz, 2H, ArH), 9.15 (d, *J* 7.5 Hz, 1H, ArH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 109.9, 115.6, 115.8, 120.3, 121.9, 124.6, 127.3, 127.7, 127.8, 131.4, 133.4, 133.4, 135.6, 167.1, 190.1 ppm. Anal. Calcd for $C_{17}H_9FN_2O_2S$ (324.33): C, 62.96; H, 2.80; N, 8.64. Found: C, 62.91; H, 2.77; N, 8.70 %.

5-[(Hydroxy)(*p*-tolyl)methylene]-2,2-dimethyl-1,2,3,5-tetrahydro-4*H*-[1,3]benzothiazolo[3,2-*a*]quinazolin-4-one (**6a**)**.** White solid. mp = 334-336 °C. IR ν/cm^{-1} (KBr): 1638, 1506, 1482; ^{1}H NMR (500 MHz, DMSO): δ 1.14 (s, 3H, CH_3), 1.18 (s, 3H, CH_3), 2.28 (s, 3H, CH_3), 2.35 (bs, 2H, CH_2, 2.72 (bs, 2H, CH_2), 7.13 (d, *J* 7.5 Hz, 2H, ArH), 7.34 (t, *J* 7.5 Hz, 1H, ArH), 7.41 (t, *J* 7.5 Hz, 1H, ArH), 7.44 (d, *J* 7.5 Hz, 1H, ArH), 7.53 (d, *J* 7.5 Hz, 2H, ArH), 7.98 (d, *J* 7.5 Hz, 1H, ArH), 11.42 (bs, 1H, OH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 21.2, 27.3, 30.0, 31.9, 79.6, 105.1, 113.3, 116.3, 124.8, 125.1, 126.5, 126.9, 129.1, 129.6, 132.5, 133.2, 136.3, 144.5, 146.5, 191.1 ppm. Anal. Calcd for $C_{24}H_{22}N_2O_2S$ (402.51): C, 71.62; H, 5.51; N, 6.96. Found: C, 71.57; H, 5.50; N, 6.93 %.

5-[(Hydroxy)(4-chlorophenyl)methylene]-2,2-dimethyl-1,2,3,5-tetrahydro-4*H*-[1,3]benzothiazolo[3,2-*a*]quinazolin-4-one (**6b**)**.** White solid. mp = 333-335 °C. IR ν/cm^{-1} (KBr): 1657, 1595, 1509; ^{1}H NMR (500 MHz, DMSO): δ 1.14 (s, 3H, CH_3), 1.19 (s, 3H, CH_3), 2.40 (d, *J* 16.0 Hz, 2H, CH_2), 2.73 (d, *J* 16.0 Hz, 2H, CH_2), 7.35- 7.48 (m, 5H, ArH), 7.65 (d, *J* 7.5 Hz, 2H, ArH), 7.98 (d, *J* 7.5 Hz, 1H, ArH), 11.51 (bs, 1H, OH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 27.5, 29.8, 31.9, 77.9, 104.7, 113.5, 117.3, 125.1, 125.2, 127.0, 128.2, 128.6, 129.6, 131.7, 133.1, 134.2, 143.2, 146.9, 195.2 ppm.

5-[(Hydroxy)(4-bromophenyl)methylene]-2,2-dimethyl-1,2,3,5-tetrahydro-4*H*-[1,3]benzothiazolo[3,2-*a*]quinazolin-4-one (**6c**)**.** White solid. mp = 331-333 °C. IR ν/cm^{-1} (KBr): 1658, 1609, 1493; ^{1}H NMR (500 MHz, DMSO): δ 1.15 (s, 3H, CH_3), 1.20 (s, 3H, CH_3), 2.49 (d, *J* 16.0 Hz, 2H, CH_2), 2.72 (d, *J* 16.0 Hz, 2H, CH_2), 7.36 (t, *J* 7.5 Hz, 1H, ArH), 7.43 (t, *J* 7.5 Hz, 1H, ArH), 7.47 (d, *J* 7.5 Hz, 1H, ArH), 7.53 (d, *J* 7.5 Hz, 2H, ArH), 7.59 (d, *J* 7.5 Hz, 2H, ArH), 7.98 (d, *J* 7.5 Hz, 1H, ArH), 11.51 (bs, 1H, OH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 27.5, 29.8, 31.9, 72.2, 104.7, 113.5,

117.3, 120.2, 125.1, 125.2, 127.0, 128.5, 129.6, 131.5, 133.1, 134.5, 143.2, 146.9, 190.9 ppm. Anal. Calcd for $C_{23}H_{19}BrN_2O_2S$ (467.38): C, 59.11; H, 4.10; N, 5.99. Found: C, 59.17; H, 4.13; N, 5.97 %.

5-[(Hydroxy)(4-methoxyphenyl)methylene]-2,2-dimethyl-1,2,3,5-tetrahydro-4*H*-[1,3]benzothiazolo[3,2-*a*]quinazolin-4-one (**6d**). White solid. mp = 337-339 °C. IR ν/cm^{-1} (KBr): 1657, 1609, 1493; ^{1}H NMR (500 MHz, DMSO): δ 1.14 (s, 3H, CH_3), 1.18 (s, 3H, CH_3), 2.36 (bs, 2H, CH_2), 2.71 (bs, 2H, CH_2), 3.74 (s, 3H, OCH_3), 6.89 (d, *J* 8.5 Hz, 2H, ArH), 7.32- 7.44 (m, 3H, ArH), 7.56 (d, *J* 8.5 Hz, 2H, ArH), 7.96 (d, *J* 7.5 Hz, 1H, ArH), 11.36 (bs, 1H, OH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 27.4, 29.9, 31.9, 55.5, 73.8, 105.1, 113.2, 114.0, 115.7, 124.7, 125.1, 126.9, 127.8, 127.9, 129.5, 133.2, 144.3, 146.4, 158.6, 194.5 ppm. Anal. Calcd for $C_{24}H_{22}N_2O_3S$ (418.51): C, 68.88; H, 5.30; N, 6.69. Found: C, 68.71; H, 5.27; N, 6.65 %.

5-[(Hydroxy)(4-fluorophenyl)methylene]-2,2-dimethyl-1,2,3,5-tetrahydro-4*H*-[1,3]benzothiazolo[3,2-*a*]quinazolin-4-one (**6e**). White solid. mp = 339-341 °C. IR ν/cm^{-1} (KBr): 1688, 1595, 1510; ^{1}H NMR (500 MHz, DMSO): δ 1.12 (s, 3H, CH_3), 1.18 (s, 3H, CH_3), 2.48 (bs, 2H, CH_2), 2.73 (bs, 2H, CH_2), 7.17-7.98 (m, 8H, ArH), 11.52 (bs, 1H, OH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 27.4, 29.9, 31.9, 84.8, 104.8, 113.4, 115.5, 116.7, 125.0, 125.2, 127.0, 128.5, 129.6, 131.8, 133.1, 143.5, 146.7, 160.6, 192.9 ppm.

5-[(Hydroxy)(4-nitrophenyl)methylene]-2,2-dimethyl-1,2,3,5-tetrahydro-4*H*-[1,3]benzothiazolo[3,2-*a*]quinazolin-4-one (**6f**). White solid. mp = 343-345 °C. IR ν/cm^{-1} (KBr): 1657, 1595, 1509; ^{1}H NMR (500 MHz, DMSO): δ 1.18 (s, 3H, CH_3), 1.21 (s, 3H, CH_3), 2.45 (bs, 2H, CH_2), 2.72 (bs, 2H, CH_2), 7.39 (t, *J* 7.5 Hz, 1H, ArH), 7.45 (t, *J* 7.5 Hz, 1H, ArH), 7.50 (d, *J* 8.0 Hz, 1H, ArH), 7.90 (d, *J* 8.5 Hz, 2H, ArH), 8.02 (d, *J* 8.0 Hz, 1H, ArH), 8.22 (d, *J* 8.5 Hz, 2H, ArH), 11.73 (bs, 1H, OH) ppm. ^{13}C NMR (125 MHz, DMSO): δ 27.9, 29.6, 32.0, 85.7, 104.4, 113.8, 119.7, 124.1, 125.3, 125.5, 126.9, 127.1, 129.8, 132.9, 141.8, 142.1, 146.1, 147.7, 195.8 ppm. Anal. Calcd for $C_{23}H_{19}N_3O_4S$ (433.48): C, 63.73; H, 4.42; N, 9.69. Found: C, 63.82; H, 4.42; N, 9.65 %.

4-Hydroxy-2-[(hydroxy(*p*-tolyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8a**)**.** White solid. mp = 374-376°C. IR ν/cm^{-1} (KBr): 3080, 2949, 1709, 1573; ^{1}H NMR (500 MHz, DMSO): δ 2.29 (s, 3H, CH_3), 7.18 (d, *J* 8.0 Hz, 2H, ArH), 7.38 (t, *J* 7.5 Hz, 1H, ArH), 7.48 (t, *J* 7.5 Hz, 1H, ArH), 7.59-7.60 (m, 3H, ArH), 7.99 (d, *J* 8.0 Hz, 1H, ArH), 10.88 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 21.2, 79.7, 113.7, 125.2, 125.2, 126.3, 127.2, 129.3, 129.4, 129.6, 131.3, 133.3, 136.8, 146.7, 151.0, 163.3, 172.3 ppm. Anal. Calcd for $C_{19}H_{15}N_3O_3S$ (365.41): C, 62.45; H, 4.14; N, 11.50. Found: C, 62.57; H, 4.17; N, 11.47 %.

4-Hydroxy-2-[(hydroxy(4-methoxyphenyl)methylene]-2H-pyrimido[2,1-b][1,3]benzothiazole-3-carboxamide (**8b**)**.** White solid. mp = 385-387 °C. IR ν/cm^{-1} (KBr): 3184, 2946, 1709, 1568; ^{1}H NMR (500 MHz, DMSO): δ 3.75 (s, 3H, OCH_3), 6.95 (d, *J* 9.0 Hz, 2H, ArH), 7.38 (t, *J* 7.5 Hz, 1H, ArH), 7.48 (t, *J* 7.5 Hz, 1H, ArH), 7.60 (d, *J* 8.0 Hz,1H, ArH), 7.64 (d, *J* 9.0 Hz, 2H, ArH), 8.00 (d, *J* 8.0 Hz, 1H, ArH), 10.81 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 55.5, 79.5, 109.9, 113.7, 114.3, 125.2, 125.2, 126.5, 127.3, 127.7, 129.5, 133.3, 146.5, 151.1, 159.0, 163.4, 172.4 ppm. Anal. Calcd for $C_{19}H_{15}N_3O_4S$ (381.41): C, 59.83; H, 3.96; N, 11.02. Found: C, 59.77; H, 3.94; N, 11.07 %.

4-Hydroxy-2-[(hydroxy(3,4-dimethoxyphenyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8c**)**.** White solid. mp = 348-350 °C. IR ν/cm^{-1} (KBr): 3403, 2835, 1698, 1590; ^{1}H NMR (500 MHz, DMSO): δ 3.74 (s, 3H, OCH_3), 3.74 (s, 3H, OCH_3), 6.96 (d, *J* 8.5 Hz, 1H, ArH), 7.23 (d, *J* 8.5 Hz, 1H, ArH), 7.36-7.41 (m, 2H, ArH), 7.49 (t, *J* 8.5 Hz, 1H, ArH), 7.64 (d, *J* 8.0 Hz, 1H, ArH), 8.01 (d, *J* 8.0 Hz, 1H, ArH), 10.86 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 55.5, 55.9, 79.4, 110.2, 112.3, 113.9, 115.7, 118.8, 125.2, 125.3, 126.3, 127.3, 129.5, 133.2, 146.4, 148.6, 148.8, 151.1, 163.5, 172.4 ppm. Anal. Calcd for $C_{20}H_{17}N_3O_5S$ (411.43): C, 58.39; H, 4.16; N, 10.21. Found: C, 58.47; H, 4.17; N, 10.16 %.

4-Hydroxy-2-[(hydroxy(4-chlorophenyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8d**)**.** White solid. mp = 367-369 °C. IR ν/cm^{-1} (KBr): 3419, 3072, 1687, 1588; ^{1}H NMR (500 MHz, DMSO): δ 6.52 (bs, 2H, 2OH), 7.37-7.49 (m, 4H, ArH), 7.59 (d, *J* 10.0 Hz, 1H, ArH), 7.73 (d, *J* 8.5 Hz, 2H, ArH), 8.01 (d, *J* 8.0 Hz, 1H, ArH), 11.07 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 79.9, 113.6, 116.0, 125.2, 125.3, 127.2, 127.9, 128.9, 129.6, 132.0, 133.2, 133.4, 143.4, 147.3, 150.9, 163.2 ppm.

4-Hydroxy-2-[(hydroxy(4-bromophenyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8e**)**.** White solid. mp = 383-385 °C. IR ν/cm^{-1} (KBr): 3307, 2844, 1695, 1603; ^{1}H NMR (500 MHz, DMSO): δ 7.38 (t, *J* 8.5 Hz, 1H, ArH), 7.47 (t, *J* 8.5 Hz, 1H, ArH), 7.57-7.60 (m, 3H, AH), 7.66 (d, *J* 8.5 Hz, 2H, ArH), 8.01 (d, *J* 8.5 Hz, 1H, ArH), 11.30 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 79.9, 113.6, 116.0, 120.6, 125.2, 127.2, 128.2, 129.7, 131.8, 133.2, 133.8, 143.4, 147.3, 150.9, 163.1, 172.4 ppm.

4-Hydroxy-2-[(hydroxy(4-nitrophenyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8f**). Yellow solid. mp = 382-384 °C. IR ν/cm^{-1} (KBr): 3207, 3022, 1706, 1598; ^{1}H NMR (500 MHz, DMSO): δ 5.79 (bs, 2H, 2OH), 7.41 (t, *J* 8.5 Hz, 1H, AH), 7.49 (t, *J* 8.5 Hz, 1H, ArH), 7.61 (d, *J* 8.5 Hz, 1H, ArH), 8.00 (d, *J* 9.5 Hz, 2H, AH), 8.03 (d, *J* 8.5 Hz, 1H, ArH), 8.26 (d, *J* 9.5 Hz, 2H, ArH), 11.82 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 79.8, 113.8, 118.3, 124.4, 125.3, 125.5, 126.7, 127.3, 129.8, 133.1, 141.5, 142.8, 146.1, 148.1, 150.9, 163.1 ppm. Anal. Calcd for $C_{18}H_{12}N_4O_5S$ (396.38): C, 54.54; H, 3.05; N, 14.14. Found: C, 54.58; H, 3.06; N, 14.08 %.

4-Hydroxy-2-[(hydroxy(4-fluorophenyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8g**). White solid. mp = 371-373 °C. IR ν/cm^{-1} (KBr): 3408, 3035, 1704, 1661; ^{1}H NMR (500 MHz, DMSO): 4.58 (bs, 2H, 2OH), 7.23 (t, *J* 7.5 Hz, 2H, ArH), 7.39 (t, *J* 8.0 Hz, 1H, ArH), 7.48 (t, *J* 8.0 Hz, 1H, ArH), 7.59 (d, *J* 8.0 Hz, 1H, ArH), 7.74 (dd, *J* 7.5 Hz, 2H, ArH), 8.02 (d, *J* 8.0 Hz, 1H, ArH), 11.84 (bs,2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 79.8, 113.6, 115.8, 125.2, 127.2, 128.2, 128.3, 129.6, 131.1, 133.3, 143.6, 147.0, 150.9, 160.7, 162.7, 163.2 ppm. Anal. Calcd for $C_{18}H_{12}FN_3O_3S$ (369.37): C, 58.53; H, 3.27; N, 11.38. Found: C, 58.57; H, 3.29; N, 11.34 %.

4-Hydroxy-2-[(hydroxy(3-nitrophenyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8h**). Yellow solid. mp = 375-377 °C. IR ν/cm^{-1} (KBr): 3118, 2961, 1676, 1574; ^{1}H NMR (500 MHz, DMSO): δ 7.40 (t, *J* 7.5 Hz, 1H, ArH), 7.49 (t, *J* 7.5 Hz, 1H, ArH), 7.63 (d, *J* 7.5 Hz, 1H, ArH), 7.69 (t, *J* 7.5 Hz,1H, AH), 8.03 (d, *J* 8.0 Hz, 1H, ArH), 8.10 (d, *J* 8.5 Hz, 1H, ArH), 8.14 (d, *J* 8.0 Hz, 1H, ArH), 8.57 (t, *J* 9.0 Hz, 1H, ArH), 11.18 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO):

79.7, 113.8, 117.2, 120.4, 121.7, 125.2, 125.4, 127.2, 129.8, 130.6, 132.1, 133.1, 136.5, 142.5, 147.7, 148.5, 150.9, 163.2 ppm.

4-Hydroxy-2-[(hydroxy(phenyl)methylene]-2*H*-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxamide (**8i**)**.** White solid. mp = 357-359 ^{o}C. IR ν/cm^{-1} (KBr): 3390, 2967, 1684, 1580; ^{1}H NMR (500 MHz, DMSO): δ 5.60 (bs, 2H, 2OH), 7.26 (t, *J* 7.5 Hz, 1H, ArH), 7.37-7.41 (m, 3H, ArH), 7.49 (t, *J* 7.5 Hz, 1H, ArH), 7.61 (d, *J* 7.5 Hz, 1H, ArH), 7.73 (d, *J* 7.5 Hz, 2H, ArH), 8.03 (d, *J* 8.0 Hz, 1H, ArH), 11.05 (bs, 2H, NH_2) ppm. ^{13}C NMR (125 MHz, DMSO): δ 79.9, 113.6, 116.0, 125.2, 125.2, 126.3, 127.2, 127.5, 128.8, 129.6, 133.3, 134.4, 144.1, 147.0, 151.0, 163.2 ppm. Anal. Calcd for $C_{18}H_{13}N_3O_3S$ (351.38): C, 61.53; H, 3.73; N, 11.96. Found: C, 61.62; H, 3.75; N, 11.94 %.