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SUPPLEMENTARY MATERIAL TO

Synthesis, characterization and theoretical studies of novel pyrimidine derivatives as potential corrosion inhibitors

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CHARACTERISATION DATA

*Ethyl 2-[5-benzoyl-4-(3-nitrophenyl)-6-phenyl-3,4-dihydropyrimidin-2(1*H*)--ylidene]acetate (**3**)*. Yield 54 %, m.p. 210–211 °C, FTIR (KBr (cm^{-1})): 3174, 3061 (NH), 1622, 1596 (C=O). ^{1}H-NMR (400 MHz, DMSO-d_6), δ/ppm: 10.98 (*s*, 1H, NH), 10.12 (*s*, 1H, NH), 8.32–7.02 (*m*, 14H, $H_{arom.}$), 5.47 (*s*, 1H, C4H), 5.32 (*s*, 1H, =CH), 4.45 (*q*, 2H, J = 3.6Hz, OCH_2), 1.16 (*t*, 3H, J = 7.6Hz, CH_3). Anal. Calcd. for $C_{27}H_{23}N_3O_5$: C, 69.07; H, 4.94; N, 8.95. Found: C, 69.05; H, 4.96; N, 8.96.

*Ethyl 2-(5-benzoyl-4,6-diphenyl-3,4-dihydropyrimidin-2(1*H*)-ylidene)acetate (**4**)*. Yield 62 %, m.p. 203–205 °C, FTIR (KBr (cm^{-1})): 3208, 3062 (NH), 1622, 1594 (C=O). ^{1}H-NMR (400 MHz, DMSO-d_6), δ/ppm: 10.96 (*s*, 1H, NH), 10.11 (*s*, 1H, NH), 8.30–6.96 (*m*, 15H, $H_{arom.}$), 5.44 (*s*, 1H, C4H), 5.30 (*s*, 1H, =CH), 4.33 (*q*, 2H, J = 4Hz, OCH_2), 1.15 (*t*, 3H, J = 6Hz, CH_3). Anal. Calcd. for $C_{27}H_{24}N_2O_3$: C, 76.39; H, 5.70; N, 6.60. Found: C, 76.40; H, 5.71; N, 6.58.

4-*(6-Benzoyl-2-benzylidene-3-oxo-7-phenyl-2,3-dihydro-5*H*-thiazolo[3,2-*a*]-pyrimidin-5-yl)benzoic acid (**6**)*. Yield 58 %, m.p. 247–248 °C, IR (KBr (cm^{-1})): 1713, 1685, 1608 (C=O); ^{1}H-NMR (400 MHz, DMSO-d_6), δ/ppm: 12.72 (*bs*, 1H, OH), 7.91–7.10 (*m*, 19H, $H_{arom.}$), 6.41 (*s*, 1H, C4H), 4.22 (*s*, 1H, CH); ^{13}C--NMR (100 MHz, DMSO-d_6), δ/ppm: 196.1 (C=O, benzoyl), 172.5, 167.1 (C=O), 164.7, 155.2, 147.1, 144.1, 137.6, 137.4, 133.4, 133.1, 132.9, 131.1, 131.1, 130.5, 129.8, 129.7, 129.5, 129.0, 128.3, 128.2, 128.1, 120.2, 116.9, 57.6. Anal. Calcd. for $C_{33}H_{22}N_2O_4S$: C, 73.05; H, 4.09; N, 5.16. Found: C, 73.03; H, 4.10; N, 5.18.

*4-(6-Benzoyl-3-oxo-7-phenyl-2,3-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-5--yl)-N-[(phenylamino)carbonyl]benzamine (**8**)*. Yield: 34 %, m.p. 205–206 °C. IR (KBr (cm^{-1})): 1704, 1620, 1597 (C=O). ^{1}H-NMR (400 MHz, DMSO-d_6), δ/

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/ ppm: 10.92 (*bs*, 1H. NH), 10.21 (*bs*, 1H, NH), 8.0–7.1 (*m*, 19H, $H_{arom.}$), 6.4 (*s*, 1H, C4H), 3.5 (*s*, 2H, CH); ^{13}C-NMR (100 MHz, DMSO-d_6), δ /ppm: 195.8 (C=O, benzoyl), 167.1, 164.2 (C=O), 157.2 (C=O), 146.3, 135.4, 134.3, 133.2, 132.9, 131.1, 130.9, 130.4, 129.5, 129.0, 128.8, 128.4, 128.0, 127.1, 126.9, 125.4, 124.1, 120.6, 66.8, 30.8. Anal. Calcd. for $C_{33}H_{24}N_4O_4S$: C, 69.22; H, 4.22; N, 9.78. Found: C, 69.20; H, 4.21; N, 9.75.

*4-(7-Benzoyl-4-oxo-8-phenyl-3,4-dihydro-2*H*,6*H*-pyrimido[2,1-b][1,3]-thiazin-6-yl)*-N,N-*diethylbenzamide (**11**)*. Yield: 43 %, m.p. 210–211 °C. IR (KBr (cm^{-1})): 1701, 1622, 1574 (C=O). ^{1}H-NMR (400 MHz, DMSO-d_6), δ /ppm: 7.30–-7.00 (*m*, 14H, $H_{arom.}$), 6.80 (*s*, 1H, C4H), 3.81 (*m*, 4H, CH), 3.40 (*bs*, 4H, CH_2), 1.17 (*bs*, 6H, CH_3). ^{13}C-NMR (100 MHz, DMSO-d_6), δ /ppm: 195.8 (C=O, benzoyl), 171.3, 167.1, 164.2 (C=O, C=N), 157.2, 146.3, 135.4, 132.9, 130.9, 130.4, 129.5, 129.0, 128.8, 128.4, 128.0, 127.1, 126.9, 125.4, 124.1, 120.6, 66.8, 43.21, 39.20, 14.11, 12.93. Anal. Calcd. for $C_{31}H_{29}N_3O_3S$: C, 71.10; H, 5.58; N, 8.02. Found: C, 71.11; H, 5.57; N, 8.04.