SUPPLEMENTARY MATERIAL TO

S**ynthesis, characterization and electrochemical properties of novel pyrimidine derivatives as potential corrosion inhibitors agents**

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CHARACTERISATION DATA

*Ethyl 2-(5-benzoyl-4-(3-nitrophenyl)-6-phenyl-3,4-dihydropyrimidin-2(1H)-ylidene)acetate (****3****):*

Yield 54%, mp 210-211ºC, FTIR (KBr/cm‒1) 3174, 3061 cm-1 (NH). 1622 and 1596 cm-1 (C=O). 1H-NMR (400 MHz, DMSOd6) δ 10.98 (s, 1H, NH), 10.12 (s, 1H, NH), 8.32-7.02 (m, 14H, Harom.), 5.47 (s, 1H, C4H), 5.32 (s, 1H, =CH), 4.45(q, 2H, OCH2), 1.16 (t, 3H, CH3). Anal. Calcd. for C27H23N3O5: 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(1H)-ylidene)acetate (****4****):*

Yield 62%, mp 203-205ºC, FTIR (KBr/cm‒1) 3208, 3062 cm-1 (NH). 1622 and 1594 cm-1 (C=O). 1H-NMR (400 MHz, DMSOd6) δ 10.96 (s, 1H, NH), 10.11 (s, 1H, NH), 8.30-6.96 (m, 15H, Harom.), 5.44 (s, 1H, C4H), 5.30 (s, 1H, =CH), 4.33 (q, 2H, OCH2), 1.15 (t, 3H, CH3). Anal. Calcd. for C27H24N2O3: 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-3,5-dihydro-2H-thiazolo[3,2-a]pyrimidin-5-yl)benzoic acid (****6****):*

Yield 58%, mp. 247-248ᵒC, IR (KBr/cm-1): 1713, 1685, 1608 (C=O); 1H NMR (400 MHz, DMSOd6) δ 12.72 (bs, 1H, OH), 7.91-7.10 (m, 19H, Harom.), 6.41 (s, 1H, C4H), 4.22 (s, 1H, CH), 13C-NMR (100 MHz, DMSOd6) δ 196.1 (C=O, benzoyl), 172.5 and 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 ppm. Anal. Calcd. for C33H22N2O4S: C, 73.05; H, 4.09; N, 5.16. Found: C, 73.03; H, 4.10; N, 5.18.

*1-(4-(6-benzoyl-3-oxo-7-phenyl-3,5-dihydro-2H-thiazolo[3,2-a]pyrimidin-5-yl)benzoyl)-3-phenylurea (****8****):*

Yield: 34%, mp 205–206ᵒC. IR (KBr) 1704, 1620, 1597 cm-1 (C=O). 1H-NMR (400 MHz, DMSOd6) δ 10.92 (bs, 1H. NH), 10.21(bs, 1H. NH), 8.0-7.1 (m, 19H, Harom.), 6.4 (s, 1H, C4H), 3.5 ppm (s, 2H, CH). 13C-NMR (100 MHz, DMSOd6) δ 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 ppm. Anal. Calcd. for C33H24N4O4S: 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-2,3,4,6-tetrahydropyrimido[2,1-b][1,3]thiazin-6-yl)-N,N-diethylbenzamide (****11****):*

Yield: 43%, mp 210–211ᵒC. IR (KBr) 1701, 1622, 1574 cm-1 (C=O). 1H-NMR (400 MHz, DMSOd6) δ 7.30-7.00 (m, 14H, Harom.), 6.80 (s, 1H, C4H), 3.81 (m, 4H, CH), 3.40 (bs, 4H, CH2), 1.17 (bs, 6H, CH3). 13C-NMR (100 MHz, DMSOd6) δ 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 ppm. Anal. Calcd. for C31H29N3O3S: C, 71.10; H, 5.58; N, 8.02. Found: C, 71.11; H, 5.57; N, 8.04.