Supplementary information

One-pot synthesis of Benzopyrano-pyrimidine derivatives catalyzed by p-toluenesulphonic acid and their Nematicidal and Molecular docking study

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Spectral data of synthesized compounds

4-nitro-2-(4-(piperidin-1-yl)-5H-chromeno[2,3-d] pyrimidin-2-yl) phenol (1)

Compound **1** crystalized from chloroform-ethanol as light brown solid. Yield 95 %, m.p 260-262°C. Anal. Calc. for $C_{22}H_{19}N_5O_6$: C, 58.80; H, 4.26: N, 15.58: found: C, 58.82; H, 4.25; N, 15.60. FTIR (KBr) cm^{-1}: 3439 (OH), 1093-11009 (C-O), 1620-1660 (N=C); ^1H NMR (500 MHz, DMSO-d_6): δ 1.74 (s, 6H), 2.51 (s, 2H), 3.55 (s, 4H), 4.15 (s, 2H), 7.1-7.2 (t, J = 8.0 Hz, 1H), 7.25-7.23 (d, J = 8.0 Hz, 1H), 7.96-7.94 (d, J = 8.0 Hz, 1H), 8.24-8.16 (m, 3H), 9.2 (s, 1H), 14.2 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 24.4, 47.0, 65.8, 97.4, 109.4, 116.1, 118.2, 119.5, 122.4, 130.3, 130.4, 131.6, 135.4, 148.6, 158.5, 159.1, 162.4, 163.2; MS (ESI) m/z: 449.1 [$M^{+\bullet}$].

2-(4-(piperidin-1-yl)-5H-chromeno [2,3-d] pyrimidin-2-yl) phenol (2)

Compound **2** crystalized from chloroform-ethanol as yellow solid. Yield 94 %, m.p 170-172°C. Anal. Calc. for $C_{22}H_{21}N_3O_2$: C, 73.52: H, 5.89: N, 11.69: found: C, 73.54: H, 5.86: N, 11.71. FTIR (KBr) cm^{-1}: 3331(OH), 1100-1111(C-O), 1643 (C=N). ; ^1H NMR (500 MHz, DMSO-d_6): δ 1.70–1.82 (m, 6H), 3.43 (t, J = 4.9 Hz, 4H), 3.91 (s, 2H), 5.86 (s, 1H), 6.91 (t, J = 8.0 Hz, 1H), 6.97 (d, J = 8.0 Hz, 1H), 7.09 (t, J = 7.3 Hz, 1H), 7.16–7.27 (m, 3H), 7.34 (t, J = 7.3 Hz, 1H), 8.41 (d, J = 8.0 Hz, 1H) ppm [27]. ^{13}C NMR (125 MHz, DMSOd_6): δ 24.2, 25.5, 25.8, 49.4, 97.3, 116.9, 117.4, 118.5, 118.7, 119.4, 124.2, 128.0, 128.4, 129.1, 132.6, 150.5, 160.3, 161.8, 164.2, 165.0 ppm; MS (ESI) m/z: 359.1 [$M^{+\bullet}$].

4-chloro-2-(7-chloro-4-(piperidin-1-yl)-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (3)

Compound **3** crystalized from chloroform-ethanol as whit solid. Yield 94 %, m.p 255-256 °C. Anal. Calc. for $C_{22}H_{19}Cl_2N_3O_2$: C, 61.69; H, 4.47; Cl, 16.55; N, 9.81; O, 7.47; found: C, 61.67; H, 4.45; Cl, 16.53; N, 9.79; O, 7.45; FTIR (KBr) cm^{-1}: 3424 (OH), 1099 (C-O), 1602-1650 (C=N); ^1H NMR (400 MHz, $CDCl_3$): δ 1.73-1.81 (m, 6H), 3.43 (t, J = 4.7Hz, 4H), 3.87 (s, 2H), 6.89 (d, J = 8.8 Hz, 1H), 7.11 (d, J = 8.4 Hz, 1H), 7.19-7.28 (m, 3H), 8.35 (d, J = 3.0, Hz, 1H) [30].^{13}C NMR (100 MHz, $CDCl_3$): δ 24.2, 25.5, 25.9, 49.5, 96.9, 118.3, 119.0, 119.4, 121.0, 123.7, 128.2, 128.32, 129.3, 132.6, 149.0, 158.9, 160.9, 165.32 ppm; MS (ESI) m/z: 427.09 [$M^{+\bullet}$].

2-(4-morpholino-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (4)

Compound **4** crystalized from chloroform-ethanol as dark brown solid. Yield 94 %, m.p 220-222. Anal. Calc. for $C_{21}H_{19}N_3O_3$; C, 69.79: H, 5.30: N, 11.63: found: C, 69.77: H, 5.32: N, 11.64. FTIR (KBr) cm^{-1}: 3348.82(OH). 1013 (C-O), 1645 (C=N). ^1H NMR (400 MHz, DMSO-d6): δ 3.60 (t, 4H, J = 4.5 Hz), 3.91 (t, 4H, J = 4.5 Hz), 4.09 (s, 2H), 6.89 (s, 1H), 6.94 (t, 1H, J = 8.0 Hz), 6.90 (d, 1H, J = 8.0 Hz), 7.14 (t, 1H, J = 7.3 Hz), 7.30-7.36 (m, 3H), 7.38 (t, J = 7.3 Hz, 1H), 8.40 (d, J = 8.0 Hz, 1H) ppm [28]. ^{13}C NMR (100 MHz, DMSO-d6): δ 25.4, 49.4, 67.1, 98.7, 117.3, 118.2, 118.3, 119.3, 120.9, 125.3, 128.9, 129.8, 133.5, 151.2, 160.2, 161.9, 164.0, 164.6 ppm. MS (ESI) m/z: 361.1 [$M^{+\bullet}$].

2-(4-(1H-pyrrol-1-yl)-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (5)

Compound **5** crystalized from chloroform-ethanol as black solid. Yield 94 %, m.p 230232°C. Anal. Calc. for $C_{21}H_{15}N_3O_2$; C, 73.89.79: H, 4.43: N, 12.31: found: C, 73.87: H, 4.45: N, 12.33). FTIR (KBr) cm^{-1}: 3385 (OH), 1099 (C-O), 1642 (C=N). ^1H NMR (500 MHz, DMSO-d_6): δ 3.80 (s, 2H), 6.8-7.2 (m, 4H J=8.0 Hz), 6.9-7.5(m, 4H J= 8.0 Hz), 7.1 (d, 2H J=7.3 Hz), 6.0-6.3 (m, 2H J=7.3Hz).^{13}C NMR (125 MHz, DMSO-d_6): δ 25.2, 102.2, 107.2, 115, 116.1, 117.2, 118.1, 120.0,120.0, 122.2, 123.1, 128.1, 129, 129.3, 150.1, 152.0, 158, 165, 168 MS (ESI) m/z: 341.12 [$M^{+\bullet}$].

2,4-dichloro-6-(7,9-dichloro-4-(piperidin-1-yl)-5H-chromeno[2,3-d]pyrimidin-2yl)Phenol (6)

Compound **6** crystalized from chloroform-ethanol as black solid. Yield 93 %, m.p.: 170°C. Anal. Cal. for $C_{22}H_{17}Cl_4N_3O_2$; C, 53.15; H, 3.45; Cl, 28.52; N, 8.45; O, 6.44: found: C, 53.14; H, 3.43; Cl, 28.51; N, 8.47; O, 6.42; FTIR (KBr) cm^{-1}: 3300, 1116 (C-O), 16701690(C=N). ^1H NMR (500 MHz, DMSO-d_6): 3.4 (s, 6H), 1.4 (s, 4H), 4.2 (s, 2H), 6.4 (s,1H), 7.1 (s, 1H), 7.4 (s, 1H), 7.20 (s, 1H), 10.2 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 22.1, 23.5, 23.5, 24.2, 51, 95, 120.1, 120.4, 122.5, 122.7, 123.4, 120.5, 122.1, 122.5, 124.4, 150, 151.1, 148, 176.5 MS (ESI) m/z: 495.01 [$M^{+\bullet}$].

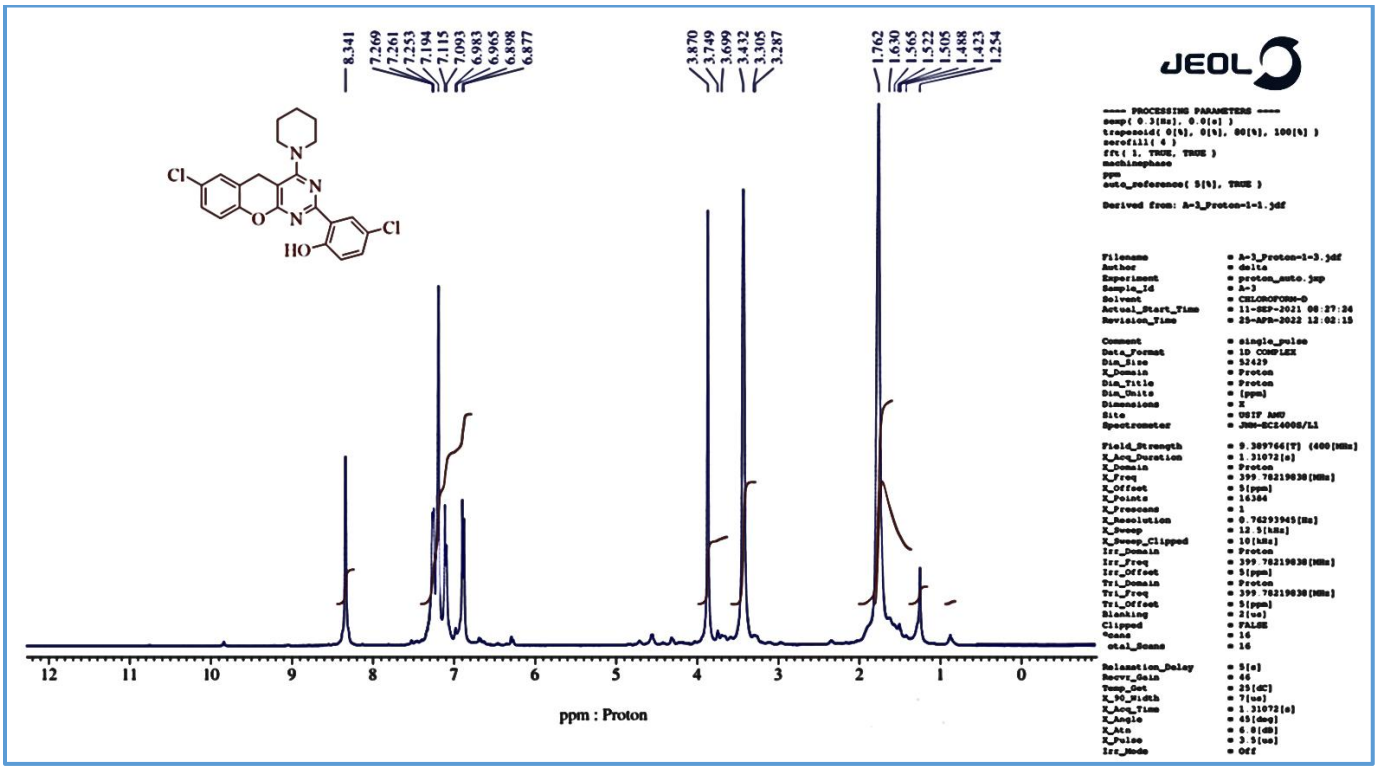

Figure S1. ^1H NMR Spectra of **Compound 3**

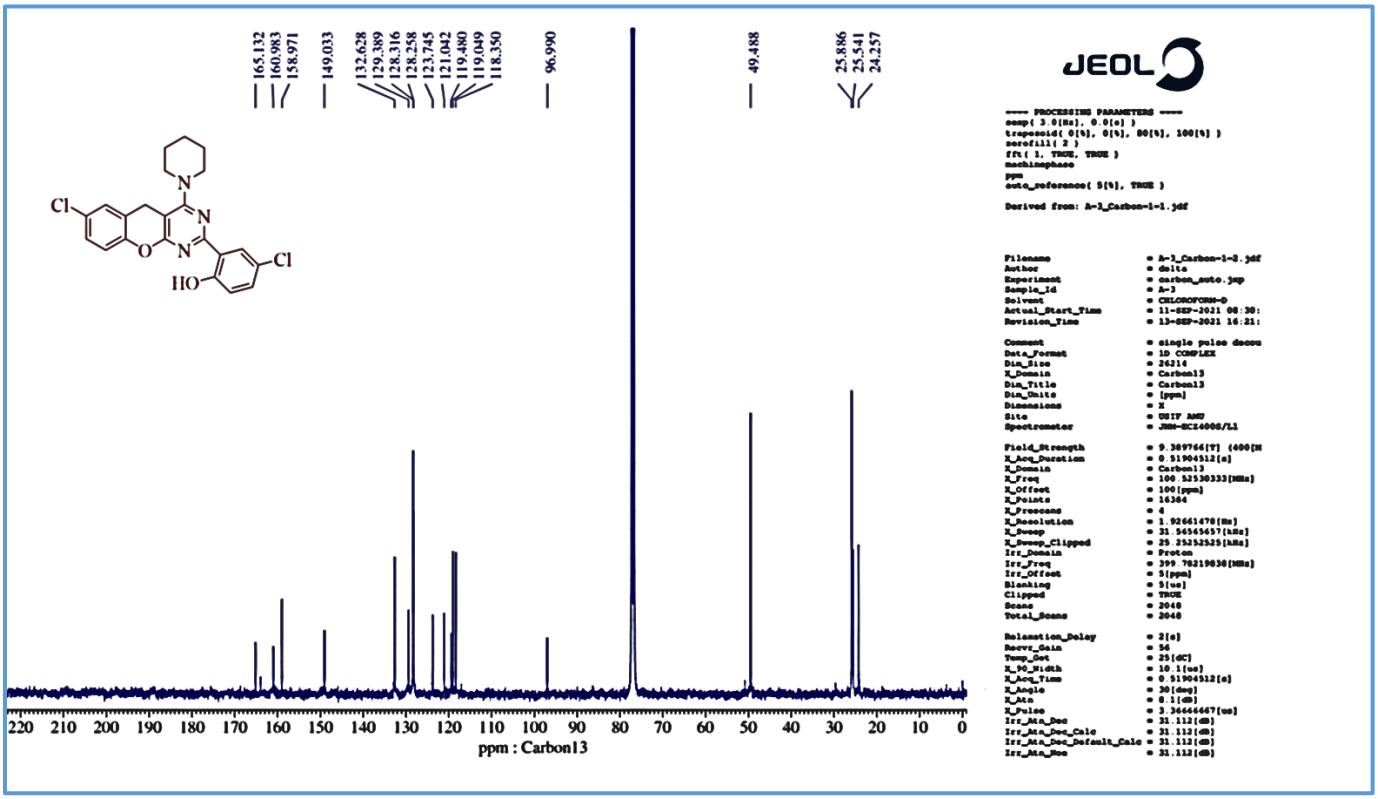

Figure S2. ^{13}C NMR Spectra of **Compound 3**

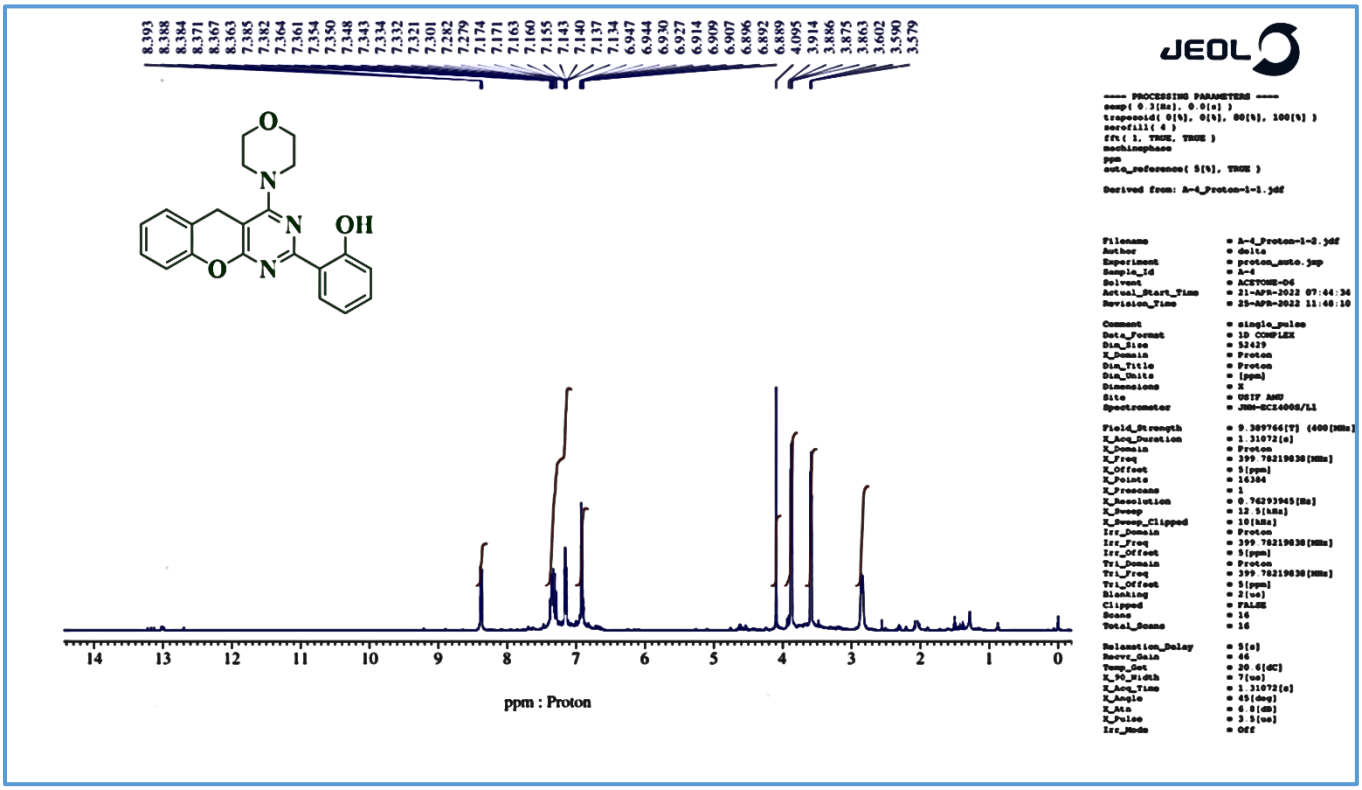

Figure S3. [1]H NMR Spectra of **Compound 4**

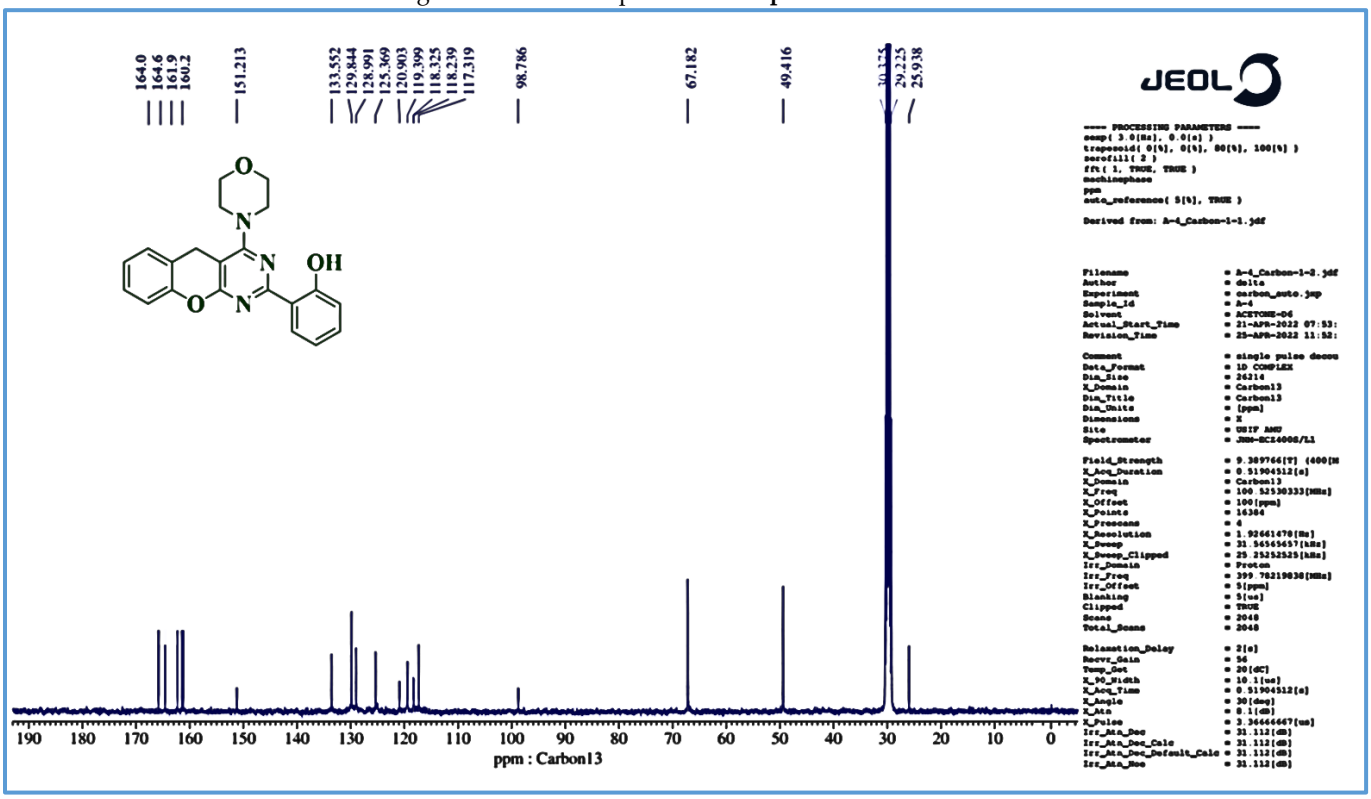

Figure S4. [13]C NMR Spectra of **Compound 4**