

Spectral and physical data of 2-amino-chromenes

- (6a)** White powder; M.P_{rep.} (°C): 233-234 (EtOH); M.P_{Lit.} (°C): 237-234 [448]; M.F: C₁₆H₁₂N₂O₂; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.17; M.W_{extract} (amu): 264.28; U.V (MeOH) λ_{\max} (nm): 278; IR (KBr) ν (cm⁻¹): 3428 (OH), 3331 (NH₂), 3216 (C=C-H), 2191 (CN), 1651 (C=C vinyl nitrile), 1587 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 4.61 (s, 1H, CH), 6.40 (d, 1H, ³J = 3 Hz, Ar-H), 6.48 (dd, 1H, ³J = 9, 3 Hz, Ar-H), 6.78 (d, 1H, ³J = 9 Hz, Ar-H), 6.86 (s, 2H, NH₂), 7.16-7.29 (m, 5H, Ar-H), 9.76 (s, 1H, OH).
- (6b)** Pale yellow powder; M.P_{rep.} (°C): 215-217 (EtOH); M.P_{Lit.} (°C): 215-217 [448]; M.F: C₁₆H₁₂N₂O₃; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.11; M.W_{extract} (amu): 280.28; U.V (MeOH) λ_{\max} (nm): 270; IR (KBr) ν (cm⁻¹): 3445 (OH), 3442 (NH₂), 3216 (C=C-H), 2194 (CN), 1651 (C=C vinyl nitrile), 1585 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 4.48 (s, 1H, CH), 6.38 (d, 1H, ³J = 2.6 Hz, Ar-H), 6.47 (dd, 1H, ³J = 9, 2.6 Hz, Ar-H), 6.51 (d, 1H, ³J = 8 Hz, Ar-H), 6.56 (d, 1H, ³J = 8.7 Hz, Ar-H), 6.61 (d, 1H, ³J = 8.7 Hz, Ar-H), 6.79 (d, 1H, ³J = 8.3 Hz, Ar-H), 6.84 (s, 2H, NH₂), 7.07 (t, 1H, ³J = 8.3 Hz, Ar-H), 9.33 (s, 1H, OH), 9.68 (s, 1H, OH); ¹³C NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 56.77, 79.63, 102.58, 112.78, 114.16, 114.28, 114.55, 118.53, 121.19, 129.92, 130.32, 148.33, 149.29, 157.49, 157.99, 160.68.
- (6c)** Yellow powder; M.P_{rep.} (°C): 218-220 (EtOH); M.P_{Lit.} (°C): 217-220 [448]; M.F: C₁₆H₁₀N₂O₂Cl₂; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.18; M.W_{extract} (amu): 333.17; U.V (MeOH) λ_{\max} (nm): 272; IR (KBr) ν (cm⁻¹): 3476 (OH), 3340 (NH₂), 3228 (C=C-H), 2192 (CN), 1643 (C=C vinyl nitrile), 1586 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 5.11 (s, 1H, CH), 6.39 (d, 1H, ³J = 2 Hz, Ar-H), 6.47 (dd, 1H, ³J = 9, 2 Hz, Ar-H), 6.70 (d, 1H, ³J = 9 Hz, Ar-H), 6.98 (s, 2H, NH₂, D₂O exchangeable), 7.19 (d, 1H, ³J = 8 Hz, Ar-H), 7.38 (dd, 1H, ³J = 8, 2, Ar-H), 7.57 (d, 1H, ³J = 2, Ar-H), 9.78 (s, 1H, OH).
- (6d)** Cream powder; M.P_{rep.} (°C): 190-192 (EtOH); M.P_{Lit.} (°C): 191-193 [448]; M.F: C₁₈H₁₆N₂O₄; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.15; M.W_{extract} (amu): 324.33; U.V (MeOH) λ_{\max} (nm): 274; IR (KBr) ν (cm⁻¹): 3434 (OH), 3343 (NH₂), 3251 (C=C-H), 2194 (CN), 1647 (C=C vinyl nitrile), 1595 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 3.68 (s, 6H, 2OCH₃), 4.52 (s, 1H, CH), 6.29 (s, 1H, Ar-H), 6.34 (s, 1H, Ar-H), 6.38 (s, 1H, Ar-H), 6.47 (d, 1H, ³J = 8.7 Hz, Ar-H), 6.83 (s, 2H, NH₂), 6.87 (d, 2H, ³J = 8.7 Hz, Ar-H), 9.96 (s, 1H, OH).
- (6e)** Pale yellow powder; M.P_{rep.} (°C): 231-232 (EtOH); M.P_{Lit.} (°C): 230-232 [448]; M.F: C₂₀H₁₄N₂O₂; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.38; M.W_{extract} (amu): 314.34; U.V (MeOH) λ_{\max} (nm): 276; IR (KBr) ν (cm⁻¹): 3482 (OH), 3413 (NH₂), 3213 (C=C-H), 2194 (CN), 1654 (C=C vinyl nitrile), 1587 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 4.77 (s, 1H, CH), 6.42 (d, 1H, ³J = 3 Hz, Ar-H), 6.44 (d, 1H, ³J = 9 Hz, Ar-H), 6.77 (d, 1H, ³J = 8.7 Hz, Ar-H), 6.91 (s, 2H, NH₂), 7.22 (d, 1H, ³J = 8.7 Hz, Ar-H), 7.47-7.72 (m, 3H, Ar-H), 7.84-7.87 (m, 3H, Ar-H), 9.7 (s, 1H, OH); ¹³C NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 56.69, 79.64, 102.77, 112.94, 113.86, 121.20, 126.02, 126.25, 126.40, 126.79, 127.98, 128.14, 129.04, 130.63, 132.51, 133.35, 144.02, 149.38, 157.69, 160.71.
- (6f)** Pale yellow crystal; M.P_{rep.} (°C): 169-172 (EtOH); M.P_{Lit.} (°C): 169-172 [448]; M.F: C₁₂H₁₂N₂O₂; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.21; M.W_{extract} (amu): 216.24; U.V (MeOH) λ_{\max} (nm): 276; IR (KBr) ν (cm⁻¹): 3444 (OH), 3344 (NH₂), 3290 (C=C-H), 2179 (CN), 1648 (C=C vinyl nitrile), 1587 (C=C aromatic); ¹H NMR (Acetone-*d*₆, 400 MHz) δ (ppm): 0.73 (t, 3H, ³J = 7 Hz, CH₃), 1.70 (q, 2H, ³J = 7 Hz, CH₂), 3.53 (s, 1H, CH), 5.98 (s, 2H, NH₂), 6.42 (d, 1H, ³J = 10 Hz, Ar-H), 6.65 (s, 1H, Ar-H), 7.06 (d, 1H, ³J = 10 Hz, Ar-H), 8.55 (s, 1H, OH).
- (7g)** Pale yellow powder; M.P_{rep.} (°C): 178-180 (EtOH); M.P_{Lit.} (°C): 179-180 [449]; M.F: C₂₀H₁₄N₂O; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.65; M.W_{extract} (amu): 298.34; U.V (MeOH) λ_{\max} (nm): 268; IR (KBr) ν (cm⁻¹): 3447 (NH₂), 3186 (C=C-H), 2202 (CN), 1656 (C=C vinyl nitrile), 1574 (C=C aromatic); ¹H NMR (Acetone-*d*₆, 400 MHz) δ (ppm): 4.93 (s, 1H, CH), 6.43 (s, 2H, NH₂), 7.15-7.33 (m, 6H, Ar-H), 7.61 (m, 3H, Ar-H), 7.89 (d, 1H, ³J = 8.2 Hz, Ar-H), 8.30 (d, 1H, ³J = 8.2 Hz, Ar-H).
- (7h)** Pale yellow powder; M.P_{rep.} (°C): 188-189 (EtOH); M.P_{Lit.} (°C): 188-189 [449]; M.F: C₂₁H₁₆N₂O₂; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.60; M.W_{extract} (amu): 328.37; U.V (MeOH) λ_{\max} (nm): 280; IR (KBr) ν (cm⁻¹): 3419 (NH₂), 3201 (C=C-H), 2192 (CN), 1661 (C=C vinyl nitrile), 1575 (C=C aromatic); ¹H NMR (Acetone-*d*₆, 400 MHz) δ (ppm): 3.47 (s, 3H, CH₃), 4.85 (s, 1H, CH), 6.38 (s, 2H, NH₂), 6.88 (d, 2H, ³J = 8.4 Hz, Ar-H), 7.11 (dd, 1H, ³J = 8.2, 6.8 Hz, Ar-H), 7.23 (d, 2H, ³J = 8.4 Hz, Ar-H), 7.58 (m, 3H, Ar-H), 7.87 (d, 1H, ³J = 8.2 Hz, Ar-H), 8.28 (d, 1H, ³J = 8.2 Hz, Ar-H).
- (7i)** Yellow powder; M.P_{rep.} (°C): 212-214 (EtOH); M.P_{Lit.} (°C): 212 [450]; M.F: C₂₀H₁₃N₃O₃; R_f (in petroleum ether:ethyl acetate; 7:3 (v/v)): 0.55; M.W_{extract} (amu): 343.34; U.V (MeOH) λ_{\max} (nm): 274; IR (KBr) ν (cm⁻¹): 3462 (NH₂), 3063 (C=C-H), 2190 (CN), 1664 (C=C vinyl nitrile), 1573 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 5.21 (s, 1H, CH), 7.15 (t, 1H, ³J = 6.8 Hz, Ar-H), 7.34 (s, 2H, NH₂), 7.60-7.67 (m, 4H, Ar-H), 7.75 (dd, 2H, ³J = 8.23, 6.8 Hz, Ar-H), 7.91 (d, 1H, ³J = 6.85 Hz, Ar-H), 8.13 (s, 1H, Ar-H), 8.26 (d, 1H, ³J = 8.3 Hz, Ar-H); ¹³C NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 55.82, 117.26, 120.69, 121.24, 122.51, 122.61, 123.31, 124.70, 126.40, 127.30, 127.49, 128.19, 130.95, 133.34, 135.06, 143.38, 148.32, 148.35, 160.89.
- (7j)** Dark gray powder; M.P_{rep.} (°C): 267-269 (EtOH); M.P_{Lit.} (°C): 266-267 [451]; M.F: C₂₀H₁₄N₂O₂; R_f (in petroleum ether:ethyl acetate; 3:2 (v/v)): 0.42; M.W_{extract} (amu): 314.34; U.V (MeOH) λ_{\max} (nm): 274; IR (KBr) ν (cm⁻¹): 3455 (OH), 3316 (NH₂), 3191 (C=C-H), 2196 (CN), 1653 (C=C vinyl nitrile), 1573 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 4.76 (s,

1H, CH), 6.70 (s, 2H, NH₂), 7.04-7.08 (m, 5H, Ar-H), 7.57-7.59 (m, 3H, Ar-H), 7.88 (d, 1H, ³J = 6.8 Hz, Ar-H), 8.23 (s, 1H, Ar-H), 9.34 (s, 1H, OH).

(8k) Pale brown powder; M.P_{rep.} (°C): 234-236 (EtOH); M.P_{Lit.} (°C): 235-236 [452]; M.F: C₂₀H₁₃N₃O₃; R_f (in petroleum ether:ethyl acetate; 3:2 (v/v)): 0.44; M.W_{extract} (amu): 339.43; U.V (MeOH) λ_{max} (nm): 268; IR (KBr) ν (cm⁻¹): 3462 (NH₂), 2190 (CN), 1668 (C=C vinyl nitrile), 1589 (C=C aromatic); ¹H NMR (DMSO-*d*₆, 400 MHz) δ (ppm): 6.06 (s, 1H, CH), 7.27 (s, 2H, NH₂), 7.87-7.91 (m, 3H, Ar-H), 8.06 (d, 1H, ³J = 7.9 Hz, Ar-H), 8.20 (dd, 1H, ³J = 8.3, 7.9 Hz, Ar-H), 8.37 (dd, 2H, ³J = 8.3, 7.9 Hz, Ar-H), 8.44 (d, 1H, ³J = 8.3 Hz, Ar-H), 8.53 (d, 1H, ³J = 8.3 Hz, Ar-H), 8.58 (s, 1H, Ar-H); ¹³C NMR (DMSO-*d*₆, 100 MHz) δ (ppm): 58.32, 114.64, 117.00, 119.70, 121.74, 121.86, 123.61, 125.24, 127.45, 128.77, 130.22, 130.29, 130.48, 131.46, 133.78, 147.53, 148.06, 148.59, 160.20.

(8l) Pale brown powder; M.P_{rep.} (°C): 174-176 (EtOH); M.P_{Lit.} (°C): 173-175 [452]; M.F: C₂₀H₁₃ClN₂O; R_f (in petroleum ether:ethyl acetate; 3:2 (v/v)): 0.58; M.W_{extract} (amu): 332.79; U.V (MeOH) λ_{max} (nm): 270; IR (KBr) ν (cm⁻¹): 3410 (NH₂), 3326 (C=C-H), 2192 (CN), 1647 (C=C vinyl nitrile), 1591 (C=C aromatic); ¹H NMR (Acetone-*d*₆, 400 MHz) δ (ppm): 5.37 (s, 1H, CH), 6.30 (s, 2H, NH₂), 7.28-7.35 (m, 5H, Ar-H), 7.45 (m, 2H, Ar-H), 7.94-7.96 (m, 3H, Ar-H).