Supplementary Data

Potassium carbonate mediated efficient and convenient synthesis of 3-Methyl-1-phenylchromeno[4,3-c]pyrazol-4(1H)-ones

Jagdeep Grover, Somendu Kumar Roy, Sanjay Madhukar Jachak*

Department of Natural Products, National Institute of Pharmaceutical Education and Research (NIPER), Sector- 67,
SAS Nagar - 160062 (Punjab), India

Tel: +91 172 2214683. Fax: +91 172 2214692. E-mail: sanjayjachak@niper.ac.in

1. Spectral data.....	2-6
2. ¹ H, ¹³ C-NMR and HRMS spectra.....	7-37

4.3.1 3-Methyl-1-phenylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (4a)^[1]: White solid; yield 95%; mp: 228–229 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.71 (s, 3H, CH₃), 7.05 (td, 1H, *J* = 1.64, 7.92 Hz, H-8), 7.12 (d, 1H, *J* = 7.7 Hz, H-9), 7.44–7.47 (m, 2H, H-6, H-7), 7.54–7.64 (m, 5H, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.9, 106.4, 111.8, 118.1, 122.4, 123.8, 126.9, 129.9, 130.1, 131.0, 139.4, 141.7, 150.8, 153.3, 158.0; HRMS (ESI) *m/z*: Calcd for C₁₇H₁₂N₂O₂Na [M+Na]⁺ 299.0796; found 299.0792.

4.3.2 3-Methyl-1-(4-(trifluoromethyl)phenyl)chromeno[4,3-*c*]pyrazol-4(1*H*)-one (4b): White solid; yield 90%; mp: 224–225 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.69 (s, 3H, CH₃), 7.10 (td, 1H, *J* = 1.56, 7.38 Hz, H-8), 7.16 (dd, 1H, *J* = 1.4, 8.2 Hz, H-9), 7.45–7.52 (m, 2H, H-6, H-7), 7.73 (d, 2H, *J* = 8.24 Hz, Ar-H), 7.89 (d, 2H, *J* = 8.32 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.8, 107.1, 111.5, 118.3, 122.2, 124.0, 127.0, 127.1, 127.2, 131.9, 141.8, 142.3, 151.5, 153.3, 157.7; HRMS (ESI) *m/z*: Calcd for C₁₈H₁₁F₃N₂O₂Na [M + Na]⁺ 367.0670; found 367.0676.

4.3.3 1-(4-Chlorophenyl)-3-methylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (4c)^[2]: White solid; yield 93%; mp: 225–226 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.70 (s, 3H, CH₃), 7.10 (t, 1H, *J* = 7.40 Hz, H-8), 7.17 (d, 1H, *J* = 7.0 Hz, H-9), 7.45–7.54 (m, 4H, Ar-H), 7.61 (d, 2H, *J* = 8.64 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.8, 106.6, 111.6, 118.2, 122.2, 124.0, 128.1, 130.1, 131.3, 136.1, 137.9, 141.8, 151.1, 153.3, 157.8; HRMS (ESI) *m/z*: Calcd for C₁₇H₁₁ClN₂O₂Na [M + Na]⁺ 333.0407; found 333.0410.

4.3.4 1-(4-Bromophenyl)-3-methylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (4d)^[2]: White solid; yield 95%; mp: 230–231 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.70 (s, 3H, CH₃), 7.11 (t, 1H, *J* = 7.40 Hz, H-8), 7.18 (d, 1H, *J* = 8.04 Hz, H-9), 7.45–7.53 (m, 4H, Ar-H), 7.77 (d, 2H, *J* = 9.10

Hz, Ar-H). ^{13}C NMR (CDCl_3 , 100 MHz): δ ppm 12.9, 106.7, 111.6, 118.2, 122.2, 124.0, 124.2, 126.9, 128.4, 131.3, 133.1, 138.3, 141.9, 151.1, 153.3, 157.8; HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{11}\text{BrN}_2\text{O}_2\text{Na}$ $[\text{M} + \text{Na}]^+$ 376.9902; found 376.9889.

4.3.5 *1-(2,4-Dichlorophenyl)-3-methylchromeno[4,3-*c*]pyrazol-4(1H)-one (4e)*: White solid; yield 90%; mp: 207–208 °C; ^1H NMR (CDCl_3 , 400 MHz): δ ppm 2.71 (s, 3H, CH_3), 6.87 (dd, 1H, $J = 1.2, 8.08$ Hz H-9), 7.11 (t, 1H, $J = 7.2$ Hz, H-8), 7.45–7.57 (m, 4H, Ar-H), 7.7 (d, 1H, $J = 1.68$ Hz, Ar-H); ^{13}C NMR (CDCl_3 , 100 MHz): δ ppm 12.9, 106.4, 111.6, 118.1, 121.5, 124.3, 128.7, 130.5, 130.7, 131.4, 133.8, 135.7, 137.3, 143.0, 151.5, 153.3, 157.6; HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}_2\text{Na}$ $[\text{M} + \text{Na}]^+$ 367.0017; found: 367.0027.

4.3.6 *1-(2,5-Dimethylphenyl)-3-methylchromeno[4,3-*c*]pyrazol-4(1H)-one (4f)*: White solid; yield 89%; mp: 186–187 °C; ^1H NMR (CDCl_3 , 400 MHz): δ ppm 1.99 (s, 3H, CH_3), 2.41 (s, 3H, CH_3), 2.70 (s, 3H, CH_3), 6.83 (d, 1H, $J = 7.96$ Hz, H-9), 7.03 (t, 1H, $J = 7.32$ Hz, H-8), 7.23 (s, 1H, Ar-H), 7.31–7.48 (m, 4H, Ar-H); ^{13}C NMR (CDCl_3 , 100 MHz): δ ppm 13.0, 16.7, 20.8, 105.6, 111.9, 117.9, 121.8, 124.2, 128.1, 131.0, 131.2, 131.4, 134.4, 137.5, 142.0, 150.6, 153.2, 158.0; HRMS (ESI) m/z : Calcd for $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_2\text{Na}$ $[\text{M} + \text{Na}]^+$ 327.1109; found. 327.1112.

4.3.7 *3-Methyl-1-(2-(trifluoromethyl)phenyl)chromeno[4,3-*c*]pyrazol-4(1H)-one (4g)*: White solid; mp: 211–212 °C; yield 91%; ^1H NMR (CDCl_3 , 400 MHz): δ ppm 2.70 (s, 3H, CH_3), 6.61 (d, 1H, $J = 8$ Hz, H-9), 6.98–7.02 (m, 1H, H-8), 7.42–7.48 (m, 2H, Ar-H), 7.57–7.59 (m, 1H, Ar-H), 7.82–7.85 (m, 2H, Ar-H), 7.97–8.00 (m, 1H, Ar-H); ^{13}C NMR (CDCl_3 , 100 MHz): δ ppm; 12.9, 106.2, 111.5, 118.1, 121.9, 124.0, 127.9, 128.0, 128.2, 128.5, 131.2, 131.3, 133.6, 136.9,

143.5, 150.8, 153.3, 157.7; HRMS (ESI) m/z : Calcd for $C_{18}H_{11}F_3N_2O_2Na$ $[M + Na]^+$ 367.0670; found 367.0677.

4.3.8 *1-(4-Fluorophenyl)-3-methylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (4h)*^[2]: White solid; yield 92%; mp: 229–230 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.68 (s, 3H, CH₃), 7.07–7.10 (m, 2H, Ar-H), 7.29–7.34 (m, 2H, Ar-H), 7.42–7.50 (m, 2H, Ar-H), 7.53–7.57 (m, 2H, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.8, 106.4, 111.7, 116.8, 117.1, 118.1, 122.2, 123.9, 128.8, 128.9, 131.2, 135.4, 141.9, 150.9, 153.3, 157.8, 161.9; HRMS (ESI) m/z : Calcd for $C_{17}H_{11}FN_2O_2Na$ $[M + Na]^+$ 317.0702; found 317.0704.

4.3.9 *7-Methoxy-3-methyl-1-phenylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (4i)*: White solid; yield 98%; mp: 206–207 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.67 (s, 3H, CH₃), 3.83 (s, 3H, OCH₃), 6.61 (dd, 1H, J = 8.96, 2.52 Hz, H-8), 6.91 (d, 1H, J = 2.48, H-6), 7.00 (d, 1H, J = 9.0 Hz, H-9), 7.52–7.61 (m, 5H, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.9, 55.6, 101.9, 104.8, 104.9, 111.8, 123.4, 123.7, 126.8, 129.8, 130.0, 131.5, 139.3, 142.1, 150.7, 155.0, 158.1, 161.8; HRMS (ESI) m/z : Calcd for $C_{18}H_{14}N_2O_3Na$ $[M + Na]^+$ 329.0902; found: 329.0906.

4.3.10 *7-Methoxy-3-methyl-1-(2-(trifluoromethyl)phenyl)chromeno[4,3-*c*]pyrazol-4(1*H*)-one (4j)*: White solid; yield 92%; mp: 193–194 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.67 (s, 3H, CH₃), 3.82 (s, 3H, OCH₃), 6.49 (d, 1H, J = 8.92 Hz, H-9), 6.57 (dd, 1H, J = 8.96, 2.48 Hz, H-8), 6.91 (d, 1H, J = 2.44, H-6), 7.54–7.57 (m, 1H, Ar-H), 7.80–7.84 (m, 2H, Ar-H), 7.95–7.97 (m, 1H, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm; 12.9, 55.6, 101.9, 104.6, 104.7, 112.1, 122.9, 127.9, 128.0, 128.6, 130.6, 131.1, 133.6, 137.0, 143.9, 150.8, 155.1, 157.9, 162.0; HRMS (ESI) m/z : Calcd for $C_{19}H_{13}F_3N_2O_3Na$ $[M + Na]^+$ 397.0776; found: 397.0779.

4.3.11 7-Methoxy-3-methyl-1-(4-(trifluoromethyl)phenyl)chromeno[4,3-*c*]pyrazol-4(1*H*)-one (**4k**): White solid; yield 96%; mp: 199–200 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.68 (s, 3H, CH₃), 3.86 (s, 3H, OCH₃), 6.68 (dd, 1H, *J* = 8.96, 2.52 Hz, H-8), 6.96 (d, 1H, *J* = 2.52 Hz, H-6), 7.08 (d, 1H, *J* = 9.0 Hz, H-9), 7.72 (d, 2H, *J* = 8.24 Hz, Ar-H), 7.89 (d, 2H, *J* = 8.36 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.8, 55.7, 102.1, 104.5, 105.5, 112.1, 123.1, 127.0, 127.1, 127.2, 142.2, 142.3, 151.5, 155.1, 157.9, 162.1; HRMS (ESI) *m/z*: Calcd for C₁₉H₁₃F₃N₂O₃Na [M + Na]⁺ 397.0776; found: 397.0776.

4.3.12 1-(4-Chlorophenyl)-7-methoxy-3-methylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (**4l**): White solid; yield 95%; mp: 266–267 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.67 (s, 3H, CH₃), 3.85 (s, 3H, OCH₃), 6.67 (dd, 1H, *J* = 9.0, 2.52 Hz, H-8), 6.94 (d, 1H, *J* = 2.48 Hz, H-6), 7.05 (d, 1H, *J* = 8.96 Hz, H-9), 7.50 (d, 2H, *J* = 8.64 Hz, Ar-H), 7.59 (d, 2H, *J* = 8.68 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.9, 55.7, 102.0, 104.7, 105.1, 112.0, 123.2, 128.1, 130.0, 137.9, 143.0, 151.1, 155.1, 158.0, 162.0; HRMS (ESI) *m/z*: Calcd for C₁₈H₁₃ClN₂O₃Na [M + Na]⁺ 363.0512; found: 363.0512.

4.3.13 1-(4-Bromophenyl)-7-methoxy-3-methylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (**4m**): White solid; yield 96%; mp: 269–270 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.67 (s, 3H, CH₃), 3.85 (s, 3H, OCH₃), 6.67 (dd, 1H, *J* = 8.96, 2.52 Hz, H-8), 6.94 (d, 1H, *J* = 2.52 Hz, H-6), 7.06 (d, 1H, *J* = 8.96 Hz, H-9), 7.44 (d, 2H, *J* = 9.48 Hz, Ar-H), 7.74 (d, 2H, *J* = 8.6 Hz, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.8, 55.7, 102.0, 104.7, 105.1, 112.0, 123.2, 124.0, 128.4, 133.0, 138.4, 142.2, 151.1, 155.1, 158.0, 162.0; HRMS (ESI) *m/z*: Calcd for C₁₈H₁₃BrN₂O₃Na [M + Na]⁺ 407.0007; found: 407.0010.

4.3.14 *1-(4-Fluorophenyl)-7-methoxy-3-methylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (4n)*: White solid; yield 90%; mp: 232–233 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 2.66 (s, 3H, CH₃), 3.84 (s, 3H, OCH₃), 6.65 (dd, 1H, *J* = 8.96, 2.56 Hz, H-8), 6.92 (d, 1H, *J* = 2.52 Hz, H-6), 6.98 (d, 1H, *J* = 8.96 Hz, H-9), 7.28–7.33 (m, 2H, Ar-H), 7.52–7.56 (m, 2H, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 12.8, 55.7, 102.0, 104.9, 112.0, 116.8, 117.0, 123.1, 128.8, 128.9, 135.4, 135.5, 142.3, 150.9, 155.0, 158.0, 162.0, 164.3; HRMS (ESI) *m/z*: Calcd for C₁₈H₁₃FN₂O₃Na [M + Na]⁺ 347.0808; found: 347.0812.

4.3.15 *1-(2,5-Dimethylphenyl)-3-methylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (4o)*: White solid; yield 88%; mp: 177–178 °C; ¹H NMR (CDCl₃, 400 MHz): δ ppm 1.99 (s, 3H, CH₃), 2.40 (s, 3H, CH₃), 2.68 (s, 3H, CH₃), 3.83 (s, 3H, OCH₃), 6.61 ((d, 1H, *J* = 8.76 Hz, H-8), 6.72 (d, 1H, *J* = 8.8 Hz, H-9), 6.93 (s, 1H, H-6), 7.23–7.32 (m, 3H, Ar-H); ¹³C NMR (CDCl₃, 100 MHz): δ ppm 13.0, 16.7, 20.8, 55.6, 101.9, 104.1, 105.1, 112.1, 122.7, 128.2, 131.2, 131.3, 132.7, 137.5, 138.1, 142.4, 150.6, 154.9, 158.3, 161.8; HRMS (ESI) *m/z*: Calcd for C₂₀H₁₈N₂O₃Na [M + Na]⁺ 357.1215; found: 357.1219.

Figure S1: ^1H NMR of compound **4a**

Figure S2: ¹³C NMR of compound **4a**

Figure S3: HRMS of compound **4a**

Figure S4: ¹H NMR of compound **4b**

Figure S5: ¹³C NMR of compound **4b**

Figure S6: HRMS of compound **4b**

Figure S7: ^1H NMR of compound **4c**

Figure S8: ¹³C NMR of compound **4c**

Figure S9: HRMS of compound **4c**

Figure S11: ¹³C NMR of compound **4d**

Figure S12: HRMS of compound **4d**

Figure S13: ¹H NMR of compound **4e**

Figure S14: ¹³C NMR of compound **4e**

Figure S15: HRMS of compound **4e**

Figure S16: ¹H NMR of compound **4f**

Figure S17: ¹³C NMR of compound **4f**

Figure S18: HRMS of compound **4f**

Figure S19: ¹H NMR of compound **4g**

Figure S20: ¹³C NMR of compound **4g**

Figure S21: HRMS of compound **4g**

Figure S22: ¹H NMR of compound **4h**

Figure S23: ¹³C NMR of compound **4h**

Figure S24: HRMS of compound **4h**

Figure S25: ¹H NMR of compound **4i**

Figure S26: ¹³C NMR of compound **4i**

Figure S27: HRMS of compound **4i**

Figure S28: ¹H NMR of compound **4j**

Figure S29: ¹³C NMR of compound **4j**

Figure 30: HRMS of compound **4j**

Figure 31: ¹H NMR of compound **4k**

Figure S32: ¹³C NMR of compound **4k**

Figure S33: HRMS of compound **4k**

Figure S34: ¹H NMR of compound **4I**

Figure S35: ¹³C NMR of compound **4l**

Figure S36: HRMS of compound **4l**

Figure S37: ¹H NMR of compound **4m**

Figure S38: ¹³C NMR of compound **4m**

Figure S39: HRMS of compound **4m**

Figure S40: ¹H NMR of compound **4n**

Figure S41: ¹³C NMR of compound **4n**

Figure S42: HRMS of compound **4n**

Figure S43: ¹H NMR of compound **4o**

Figure S44: ^{13}C NMR of compound **4o**

Figure S45: HRMS of compound **4o**

References

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