Supporting information

A one pot sequential five component domino reaction for expedient synthesis of polysubstituted pyrroles.

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Copies of \textsuperscript{1}H and \textsuperscript{13}C NMR spectra of Compounds 10-35
**General consideration**

The melting points were measured in open capillary tubes and are uncorrected. The $^1$H and $^{13}$C NMR spectra were recorded on a Bruker (Avance) 300 MHz NMR instrument using TMS as internal standard either CDCl$_3$ or DMSO-d$_6$ as solvent. Chemical shifts are given in parts per million (δ-scale) and the coupling constants are given in hertz (Hz). Silica gel-G plates (Merck) were used for thin layer chromatography (TLC) analysis with a mixture of petroleum ether (60-80 °C) and ethyl acetate as eluent. The single crystal X-ray data were collected on BRUKER GADDS X-ray (three-circle) diffractometer with Mo Kα(κ= 1.5418 A°) radiation. Elemental analyses were performed on a vario EL III CHNS elemental analyzer. Mass spectra were recorded in LCQ Fleet mass spectrometer, Thermo Fisher Instruments Limited, US. Electrospray ionization mass spectrometry (ESI-MS) analysis was performed in the positive ion and negative ion mode on a liquid chromatography ion trap.

**General procedure for the synthesis of 2-(4-benzoyl-1, 2-diphenyl-1H-pyrrol-3-yl)-2-cyanoacetamide:**

A 25 mL round bottom flask equipped with a magnetic stirrer was charged with acetonophene 1 (1.0 mmol), DMF-DMA 2 (1.0 mmol), the reaction mixture was heated on an oil bath at 100 °C for 1 h. after one hour the reaction colour was changed colourless to reddish-brown, then other reactants amine 3 (1.0 mmol), arylglyoxal 4 (1.0 mmol) and malanonitrile 5(1.0 mmol) in methanol 5mL was added reaction system, the reaction was stirred 60-70 °C for 30 min. The completion of the reaction was monitored by TLC. After completion of the reaction, the mixture was cooled to room temperature and the solid product was filtered, washed with a small portion of cold ethanol to obtain pure product 6aa-au. Analytical and spectroscopic data of the series of 2-(4-benzoyl-1, 2-diphenyl-1H-pyrrol-3-yl)-2-cyanoacetamide are given below.
4.2.1 2-(4-benzoyl-2-(4-methoxyphenyl)-1-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (6aa).

White solid, mp: 215-217 °C; $^1$H NMR (300 MHz, CDCl$_3$) δ: 7.90 (d, $J = 7.2$ Hz, 2H), 7.67 (s, 1H), 7.58 (d, $J = 6.6$ Hz, 1H), 7.53-7.48 (m, 2H), 7.36 (s, 1H), 7.29 (broad, 3H), 7.20 (d, $J = 7.5$ Hz, 2H), 7.10 (broad, 2H), 6.86 (d, $J = 7.8$ Hz, 2H), 5.77 (s, 1H), 5.10 (s, 1H), 3.80 (s, 3H) ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) δ: 191.9, 167.3, 160.1, 139.5, 138.6, 136.9, 132.5, 132.2, 131.4, 129.3, 129.3, 128.5, 128.1, 125.8, 121.7, 120.7, 116.5, 114.1, 113.2, 55.3, 36.4 ppm. MS m/z 435.48 (M$^+$+1). Anal. Calcd for C$_{27}$H$_{23}$N$_2$O$_3$: C, 74.47; H, 4.86; N, 9.65; found C, 74.41; H, 4.80; N, 9.58.

4.2.2 2-(4-benzoyl-1-(4-chlorophenyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (6ab).

White solid, mp: 238-240 °C; $^1$H NMR (300 MHz, CDCl$_3$) δ: 7.90 (d, $J = 7.8$ Hz, 2H), 7.61-7.58 (m, 2H), 7.54-7.48 (m, 3H), 7.38-7.36 (m, 4H), 7.29-7.26 (m, 3H), 7.07 (d, $J = 8.7$ Hz, 2H), 6.84 (s, 1H), 5.08 (s, 1H) ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) δ: 190.9, 166.5, 139.0, 136.7, 136.2, 133.6, 132.0, 130.8, 130.7, 129.2, 128.9, 128.8, 128.5, 128.3, 128.2, 126.7, 121.6, 116.4, 113.7, 36.0 ppm. MS m/z 439.10 (M$^+$+1). Anal. Calcd for C$_{25}$H$_{18}$ClN$_2$O$_3$: C, 70.99; H, 4.12; N, 9.55; found C, 70.92; H, 4.85; N, 9.48.

4.2.3 2-(4-benzoyl-1, 2-bis(4-chlorophenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6ac).

White solid, mp: 186-188 °C; $^1$H NMR (300 MHz, CDCl$_3$) δ: 7.89 (d, $J = 8.7$ Hz, 2H), 7.62-7.49 (m, 5H), 7.39 (s, 1H), 7.37-7.32 (m, 3H), 7.29-7.26 (m, 3H), 7.08 (d, $J = 8.7$ Hz, 2H ), 5.08 (s, 1H) ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) δ: 190.6, 166.1, 138.9, 136.6, 136.0, 133.4, 131.7, 130.6, 129.0, 128.7, 128.6, 128.3, 128.1, 126.7, 121.4, 116.3, 113.6, 35.8 ppm. MS m/z 474.34 (M$^+$+1). Anal. Calcd for C$_{26}$H$_{17}$Cl$_2$N$_2$O$_3$: C, 65.84; H, 3.61; N, 8.86; found C, 65.79; H, 3.55; N, 8.80.

4.2.4 2-(4-benzoyl-1-(3-chlorophenyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (6ad).

White solid, mp: 188-190 °C; $^1$H NMR (300 MHz, CDCl$_3$) δ: 7.90 (d, $J = 6.9$ Hz, 2H), 7.60-7.49 (m, 5H), 7.37 (broad, 4H), 7.28-7.26 (m, 3H), 7.20 (d, $J = 8.1$ Hz, 1H), 6.91 (d, $J = 7.2$ Hz, 1H), 5.82 (s, 1H), 5.05 (s, 1H) ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) δ: 191.7, 166.9, 139.5, 139.3, 136.8, 135.0, 132.4, 131.1, 130.3, 129.4, 129.2, 128.9, 128.6, 128.4, 128.3, 125.8, 124.2, 122.1, 116.4, 114.0, 36.2 ppm.
MS m/z 439.10 (M^+1). Anal. Calcd for C_{20}H_{18}ClN_{2}O_{2}: C, 70.99; H, 4.12; N, 9.55; found C, 70.92; H, 4.06; N, 9.48.

4.2.5 2-(1-(3-chlorophenyl)-4-(4-methoxybenzoyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (6ae).
White solid, mp: 170-173 °C; ^1H NMR (300 MHz, CDCl_3) δ: 7.93 (d, J = 8.7 Hz, 2H), 7.38-7.36 (m, 4H), 7.28-7.26 (m, 4H), 7.20 (d, J = 7.8 Hz, 2H), 7.01 (d, J = 8.7 Hz, 2H), 6.91(d, J = 7.8 Hz, 1H), 5.79 (s, 1H), 5.04 (s, 1H), 3.90 (s, 3H) ppm; ^13C NMR (75 MHz, CDCl_3) δ: 191.7, 166.9, 139.5, 139.3, 136.8, 135.0, 132.4, 131.1, 130.3, 129.4, 129.2, 128.6, 128.4, 128.3, 125.8, 124.2, 122.1, 116.4, 114.0, 36.2 ppm. MS m/z 469.11 (M^+1). Anal. Calcd for C_{20}H_{20}ClN_{2}O_{2}: C, 69.01; H, 4.29; N, 8.94; found C, 69.01; H, 4.29; N, 8.94.

4.2.6 2-(2-(4-bromophenyl)-1-(3-chlorophenyl)-4-(4-methoxybenzoyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6af).
White solid, mp: 176-178 °C; ^1H NMR (300 MHz, CDCl_3) δ: 7.92 (d, J = 8.7 Hz, 2H), 7.87 (s, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.35 (s, 1H), 7.31-7.16 (m, 5H), 7.01 (d, J = 8.7 Hz, 2H), 6.89 (d, J = 7.8 Hz, 1H), 5.83 (s, 1H), 5.08 (s, 1H), 3.90 (s, 3H) ppm; ^13C NMR (75 MHz, CDCl_3) δ: 190.5, 167.0, 163.5, 139.4, 135.2, 135.1, 132.7, 132.1, 131.8, 131.6, 130.5, 128.6, 127.3, 125.9, 124.3, 124.0, 122.4, 114.4, 114.0, 55.6, 36.2 ppm. MS m/z 547.02 (M^+1). Anal. Calcd for C_{20}H_{18}BrClN_{2}O_{2}: C, 59.09; H, 3.49; N, 7.66; found C, 59.01; H, 3.43; N, 7.60.

4.2.7 2-(4-benzoyl-2-phenyl-1-(p-tolyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6ag).
White solid, mp: 225-227 °C; ^1H NMR (300 MHz, CDCl_3) δ: 7.89 (d, J = 7.8 Hz, 2H), 7.61-7.56 (m, 2H), 7.53-7.48 (m, 2H), 7.39-7.33 (m, 4H), 7.28-7.26 (m, 2H), 7.08 (d, J = 8.1 Hz, 2H), 6.97 (d, J = 8.4 Hz, 2H), 6.63 (s, 1H), 5.10 (s, 1H), 2.30 (s, 3H) ppm; ^13C NMR (75MHz, CDCl_3) δ: 191.1, 166.7, 139.1, 137.8, 136.3, 135.6, 131.8, 131.2, 130.7, 129.5, 128.8, 128.6, 128.5, 128.2, 128.2, 125.2, 121.1, 116.4, 113.1, 36.0, 20.7 ppm. MS m/z 419.16 (M^+1). Anal. Calcd for C_{27}H_{21}N_{2}O_{2}: C, 77.31; H, 5.05; N, 10.02; found C, 77.24; H, 4.99; N, 9.95.

4.2.8 2-cyano-2-(4-(4-methoxybenzoyl)-2-phenyl-1-(p-tolyl)-1H-pyrrol-3-yl)acetamide (6ah).
White solid, mp: 148-150 °C; \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\): 7.93 (d, \(J = 8.7\) Hz, 2H), 7.76 (s, 1H), 7.34-7.33 (m, 4H), 7.26 (broad, 2H), 7.07 (d, \(J = 8.1\) Hz, 2H), 6.97 (t, \(J = 7.2\) Hz, 4H), 5.78 (s, 1H), 5.06 (s, 1H), 3.89 (s, 3H), 2.31 (s, 3H) ppm; \(^1^C\) NMR (75 MHz, CDCl\(_3\)) \(\delta\): 190.6, 167.3, 153.2, 138.1, 136.5, 136.1, 132.0, 131.7, 131.2, 130.8, 129.9, 129.0, 128.8, 128.6, 125.5, 121.7, 116.5, 113.8, 113.4, 55.6, 36.4, 21.1 ppm. MS m/z 449.17 (M\(^{+}\)+1). Anal. Calcd for C\(_{23}\)H\(_2\)N\(_3\)O\(_3\): C, 74.82; H, 5.16; N, 9.35; found C, 74.75; H, 5.10; N, 9.27.

4.2.9 2-(2-(4-bromophenyl)-4-(4-methoxybenzoyl)-1-(p-tolyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6ai).

White solid, mp: 167-169 °C; \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\): 7.93 (d, \(J = 8.7\) Hz, 2H), 7.81 (s, 1H), 7.35-7.33 (m, 5H), 7.28-7.26 (m, 1H), 7.07 (d, \(J = 8.1\) Hz, 2H), 7.01-6.96 (m, 3H), 5.68 (s, 1H), 5.07 (s, 1H), 3.89 (s, 3H), 2.31 (s, 3H) ppm; \(^1^C\) NMR (75 MHz, CDCl\(_3\)) \(\delta\): 190.6, 167.3, 163.2, 138.1, 136.6, 136.1, 132.0, 131.7, 131.2, 130.8, 129.9, 129.0, 128.9, 128.6, 125.6, 121.8, 113.8, 113.5, 55.6, 36.4, 21.1 ppm. MS m/z 527.08 (M\(^{+}\)+1). Anal. Calcd for C\(_{25}\)H\(_{20}\)BrN\(_3\)O\(_3\): C, 63.65; H, 4.20; N, 7.95; found C, 63.61; H, 4.15; N, 7.91.

4.2.10 2-(4-benzoyl-1-(3,5-dichlorophenyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (6aj).

White solid, mp: 163-165 °C; \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\): 7.89 (d, \(J = 7.2\) Hz, 2H), 7.62-7.28 (m, 11H), 6.99 (s, 2H), 5.94 (s, 1H), 5.037 (s, 1H) ppm; \(^1^C\) NMR (75 MHz, CDCl\(_3\)) \(\delta\): 191.5, 166.8, 140.0, 139.0, 136.7, 135.5, 132.4, 131.0, 130.7, 129.6, 129.2, 129.0, 128.6, 128.4, 127.8, 124.3, 122.3, 116.2, 114.2, 36.0 ppm. MS m/z 474.34 (M\(^{+}\)+1). Anal. Calcd for C\(_{29}\)H\(_{17}\)Cl\(_2\)N\(_3\)O\(_2\): C, 65.84; H, 3.61; N, 8.86; found C, 65.80; H, 3.56; N, 8.81.

4.2.11 2-(4-benzoyl-2-(4-chlorophenyl)-1-(3-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6ak).

White solid, mp: 195-197 °C; \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\): 7.89(d, \(J = 7.5\) Hz, 2H), 7.70 (s, 1H), 7.59 (d, \(J = 6.3\) Hz, 1H), 7.54-7.49 (m, 2H), 7.38 (s, 1H), 7.34 (d, \(J = 8.4\) Hz, 2H), 7.27-7.19 (m, 3H), 6.84 (d, \(J = 8.4\) Hz, 1H), 6.67 (d, \(J = 7.8\) Hz, 1H), 6.58 (s, 1H), 5.80 (s, 1H), 5.10 (s, 1H), 3.67 (s, 3H)
ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$: 191.9, 167.0, 160.2, 139.4, 139.3, 135.5, 132.5, 132.3, 131.7, 130.2, 129.2, 129.0, 128.6, 127.2, 121.8, 118.0, 116.2, 114.0, 113.9, 111.9, 55.5, 36.2 ppm. MS m/z 469.11 (M$^+$+1). Anal. Calcd for C$_{27}$H$_{26}$ClN$_3$O$_3$: C, 69.01; H, 4.29; N, 8.94; found C, 68.97; H, 4.25; N, 8.89.

4.2.12 2-(4-benzyloxy-2-(4-chlorophenyl)-1-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6al).

White solid, mp: 203-205 °C; $^1$H NMR (300 MHz, CDCl$_3$) $\delta$: 7.89 (d, $J = 7.2$ Hz, 2H), 7.73 (s, 1H), 7.58 (d, $J = 7.2$ Hz, 1H), 7.53–7.48 (m, 2H), 7.33 (s, 1H), 7.32 (d, $J = 7.2$ Hz, 2H), 7.26-7.22 (m, 2H), 7.01 (d, $J = 8.9$ Hz, 2H), 6.80 (d, $J = 8.9$ Hz, 2H), 5.82 (s, 1H), 5.11 (s, 1H), 3.78 (s, 3H) ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$: 191.8, 167.3, 159.3, 139.3, 135.6, 135.2, 132.5, 132.3, 131.9, 131.0, 129.2, 128.8, 128.5, 127.0, 121.4, 116.2, 114.5, 113.4, 55.5, 36.2 ppm. MS m/z 469.11 (M$^+$+1). MS m/z 469.11 (M$^+$+1). Anal. Calcd for C$_{27}$H$_{26}$ClN$_3$O$_3$: C, 69.01; H, 4.29; N, 8.94; found C, 68.97; H, 4.26; N, 8.91.

4.2.13 2-(4-benzyloxy-2-(4-chlorophenyl)-1-(2-hydroxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6am).

Brown solid, mp: 155-157 °C; $^1$H NMR (300 MHz, CDCl$_3$) $\delta$: 7.84 (d, $J = 7.2$ Hz, 2H), 7.56-7.54 (m, 2H), 7.48–7.43 (m, 2H), 7.33 (s, 1H), 7.18 (broad, 5H), 7.09 (d, $J = 7.8$ Hz, 1H), 6.86-6.82 (m, 2H), 5.87 (s, 1H), 5.07 (s, 1H) ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$: 191.9, 168.2, 151.9, 139.0, 136.7, 135.1, 133.2, 132.3, 131.9, 130.6, 129.2, 128.7, 128.5, 127.0, 125.2, 121.2, 120.2, 117.4, 116.3, 112.2, 36.4 ppm. MS m/z 455.10 (M$^+$+1). Anal. Calcd for C$_{26}$H$_{14}$ClN$_3$O$_3$: C, 68.50; H, 3.98; N, 9.22; found C, 68.46; H, 3.95; N, 9.18.

4.2.14 2-(4-benzyloxy-2-(4-chlorophenyl)-1-(4-hydroxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6an).

White solid, mp: 148-150 °C; $^1$H NMR (300 MHz, CDCl$_3$) $\delta$: 7.85 (d, $J = 7.2$ Hz, 2H), 7.73 (s, 1H), 7.57 (t, $J = 7.2$ Hz, 1H), 7.49 (t, $J = 7.2$ Hz, 2H), 7.28-7.23 (m, 3H), 7.17 (d, $J = 8.1$ Hz, 2H), 7.10 (s,
1H), 6.87 (d, J = 8.7 Hz, 2H), 6.70 (d, J = 8.7 Hz, 2H), 5.94 (s, 1H), 5.13 (s, 1H) ppm; 13C NMR (75 MHz, CDCl3) δ: 192.0, 167.4, 156.3, 139.0, 135.6, 135.1, 132.3, 132.0, 130.3, 129.1, 128.7, 128.4, 127.0, 121.1, 116.0, 112.9, 36.1 ppm. MS m/z 455.10 (M^+1). Anal. Calcd for C26H16ClN3O3: C, 68.50; H, 3.98; N, 9.22; found C, 68.47; H, 3.94; N, 9.17.

4.2.15 2-(4-benzoyl-1-(4-hydroxyphenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6ao).

White solid, mp: 113-115 °C; 1H NMR (300 MHz, CDCl3) δ: 7.84 (d, J = 8.4 Hz, 2H), 7.54 (t, J = 7.2 Hz, 2H), 7.47 (t, J = 7.8 Hz, 2H), 7.26 (s, 1H), 7.20 (d, J = 8.4 Hz, 2H), 6.87 (d, J = 8.7 Hz, 2H), 6.79 (d, J = 9.0 Hz, 2H), 6.69 (d, J = 8.7 Hz, 2H), 5.94 (s, 1H), 5.08 (s, 1H), 3.72 (s, 3H) ppm; 13C NMR (75 MHz, CDCl3) δ: 192.2, 167.9, 160.0, 156.2, 139.3, 137.1, 132.4, 132.3, 132.3, 131.7, 131.0, 129.2, 128.5, 127.1, 121.1, 120.7, 116.0, 114.1, 112.5, 55.2, 36.6 ppm. MS m/z 451.15 (M^+1). Anal. Calcd for C27H25N3O3: C, 71.83; H, 4.69; N, 9.31; found C, 71.79; H, 4.65; N, 9.28.

4.2.16 2-(4-benzoyl-1-(4-iodophenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6ap).

White solid, mp: 225-227 °C; 1H NMR (300 MHz, CDCl3) δ: 7.88 (d, J = 8.4 Hz, 2H), 7.63-7.57 (m, 4H), 7.53-7.48 (m, 2H), 7.32 (s, 1H), 7.19 (d, J = 8.4 Hz, 2H), 6.88 (d, J = 8.7 Hz, 2H), 6.83 (d, J = 8.7 Hz, 2H), 5.81 (s, 1H), 5.06 (s, 1H), 3.82 (s, 3H) ppm; 13C NMR (75 MHz, CDCl3) δ: 191.8, 167.1, 160.3, 139.3, 138.5, 138.3, 136.7, 132.5, 132.4, 130.9, 129.3, 128.6, 127.4, 122.0, 120.3, 116.4, 114.3, 113.7, 93.5, 55.3, 36.3 ppm. MS m/z 561.05 (M^+1). Anal. Calcd for C27H20I3NO3: C, 57.77; H, 3.59; N, 7.49; found C, 57.73; H, 3.56; N, 7.45.

4.2.17 2-(4-benzoyl-1-(4-ethylphenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6aq).

White solid, mp: 167-169 °C; 1H NMR (300 MHz, CDCl3) δ: 7.89 (d, J = 7.5 Hz, 2H), 7.66 (s, 1H), 7.60-7.55 (m, 1H), 7.48 (t, J = 7.5 Hz, 2H), 7.33 (s, 1H), 7.20 (d, J = 8.1 Hz, 2H), 7.11 (d, J = 7.8 Hz, 2H), 6.99 (d, J = 7.8 Hz, 2H), 6.86 (d, J = 7.8 Hz, 2H), 5.95 (s, 1H), 5.11 (s, 1H), 3.88, (s, 3H), 2.61 (q, J = 7.5Hz, 2H), 1.17 (t, J = 7.5 Hz, 3H) ppm; 13C NMR (75 MHz, CDCl3) δ: 191.2, 167.4, 160.0, 144.3, 139.5, 136.8, 136.2, 132.1, 131.6, 129.2, 128.6, 128.5, 125.6, 121.4, 120.8, 116.5, 114.1, 113.0,
55.3, 36.4, 28.4, 15.3 ppm. MS m/z 463.18 (M^+1). Anal. Calcd for C_{29}H_{35}N_{3}O_3: C, 75.14; H, 5.44; N, 9.07; found C, 75.10; H, 5.41; N, 9.03.

4.2.18 2-(4-benzoyl-1-(4-fluorophenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6ar).

White solid, mp: 168-170 °C; H NMR (300 MHz, CDCl_3) δ: 7.89 (d, J = 7.5 Hz, 2H), 7.62-7.57 (m, 2H), 7.51 (t, J = 7.8 Hz, 2H), 7.32 (s, 1H), 7.19 (d, J = 8.4 Hz, 2H), 7.10-7.06 (m, 2H), 7.01-6.96 (m, 2H), 6.87 (d, J = 8.7 Hz, 2H), 5.87 (s, 1H), 5.08 (s, 1H), 3.80 (s, 3H) ppm; C NMR (75 MHz, CDCl_3) δ: 191.8, 167.1, 163.6, 160.3, 139.6, 137.0, 134.8, 132.6, 132.2, 131.2, 129.2, 128.6, 127.7, 127.6, 121.8, 120.5, 116.5, 116.2, 114.3, 113.5, 55.3, 36.3 ppm. MS m/z 453.14 (M^+1). Anal. Calcd for C_{27}H_{29}FN_{3}O_3: C, 71.51; H, 4.45; N, 4.19; found C, 71.47; H, 4.41; N, 4.14.

4.2.19 2-(4-benzoyl-2-(4-chlorophenyl)-1-(4-fluorophenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6as).

White solid, mp: 189-191 °C; H NMR (300 MHz, CDCl_3) δ: 7.88 (d, J = 7.5 Hz, 2H), 7.62-7.57 (m, 2H), 7.52-7.47 (m, 2H), 7.35 (s, 1H), 7.32 (d, J = 8.7 Hz, 2H), 7.23 (d, J = 7.8 Hz, 2H), 7.11-7.06 (m, 2H), 7.01 (d, J = 7.8 Hz, 2H), 6.30 (s, 1H), 5.14 (s, 1H) ppm; C NMR (75 MHz, CDCl_3) δ: 191.7, 167.1, 163.6, 160.3, 139.1, 135.5, 135.5, 134.3, 134.2, 132.5, 132.4, 131.6, 129.2, 129.0, 128.5, 127.7, 127.6, 126.8, 121.7, 116.6, 116.3, 116.1, 113.9, 36.1 ppm. MS m/z 457.09 (M^+1). Anal. Calcd for C_{29}H_{17}ClF_{3}N_{3}O_3: C, 68.20; H, 3.74; N, 9.18; found C, 74.78; H, 5.12; N, 9.31.

4.2.20 2-(4-benzoyl-1-benzyl-2-(4-chlorophenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (6at).

White solid, mp: 213-215 °C; H NMR (300 MHz, CDCl_3) δ: 7.82 (d, J = 7.8 Hz, 2H), 7.67 (s, 1H), 7.61-7.56 (m, 1H), 7.49 (d, J = 7.8 Hz, 2H), 7.42 (t, J = 7.8 Hz, 3H), 7.32-7.26 (m, 4H), 7.21 (s, 1H), 6.90 (m, 2H), 5.58 (s, 1H), 5.08 (s, 1H), 4.95 (s, 2H) ppm; C NMR (75 MHz, CDCl_3) δ: 191.4, 166.7, 139.1, 135.8, 135.7, 135.3, 132.6, 132.1, 130.7, 129.1, 128.8, 128.3, 128.0, 126.7, 126.6, 120.6, 116.1, 113.2, 51.4, 35.9 ppm. MS m/z 453.92 (M^+1). Anal. Calcd for C_{27}H_{36}ClN_{3}O_{3}: C, 71.44; H, 4.44; N, 9.26; found C, 71.40; H, 4.41; N, 9.22.
4.2.21 2-(4-(5-bromo thiophene-2-carbonyl)-2-phenyl-1-(p-tolyl)-1H-pyrrol-3-yl)-2-cyanoacetamide
(6au).

White solid, mp; 163-165 °C; $^1$H NMR (300 MHz, CDCl$_3$) $\delta$: 7.66-7.65 (m, 2H), 7.52 (s, 1H), 7.35-7.33 (m, 3H), 7.24-7.19 (m, 3H), 7.12 (d, $J = 8.4$ Hz, 2H), 7.02 (d, $J = 8.4$ Hz, 2H), 6.92 (s, 1H), 4.98 (s, 1H), 2.33 (s, 3H) ppm; $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$: 180.3, 166.3, 145.5, 137.9, 135.6, 132.7, 130.9, 130.7, 129.6, 129.1, 128.7, 128.5, 128.2, 125.3, 120.5, 116.3, 113.2, 36.0, 20.7 ppm. MS m/z 504.40 (M$^+$+1). Anal. Calcd for C$_{25}$H$_{18}$BrN$_3$O$_2$S: C, 59.53; H, 3.60; N, 8.33; found C, 59.48; H, 3.57; N, 8.29.
$^1$H spectrum of 6aa.

$^{13}$C NMR Spectrum of 6aa.
$^1$H spectrum of 6ab.

$^{13}$C NMR Spectrum of 6ab.
ESI-MASS Spectrum of 6ab.

$^1$H spectrum of 6ac.
$^{13}$C NMR Spectrum of $6\text{ac}$. 

$^1$H spectrum of $6\text{ad}$.
\[ ^{13}\text{C} \text{NMR Spectrum of 6ad.} \]

ESI-MASS Spectrum of 6ad.
$^1$H spectrum of 6ae.

$^{13}$C NMR Spectrum of 6ae.
ESI-MASS Spectrum of 6ae.

\(^1\)H NMR Spectrum of 6af.
$^{13}$C NMR Spectrum of 6af.

ESI-MASS Spectrum of 6af.
$^1$H NMR Spectrum of 6ag.

$^{13}$C NMR Spectrum of 6ag.
ESI-MASS Spectrum of 6ag.

$^1$H NMR Spectrum of 6ah.
$^{13}$C NMR Spectrum of 6ah.

ESI-MASS Spectrum of 6ah.
$^1$H NMR Spectrum of 6ai.

$^{13}$C NMR Spectrum of 6ai.
ESI-MASS Spectrum of 6ai.

$^1$H NMR Spectrum of 6aj.
$^{13}$C NMR Spectrum of 6aj.

$^1$H NMR Spectrum of 6ak.
$^{13}$C NMR Spectrum of 6ak.

$^1$H NMR Spectrum of 6al.
**$^{13}$C NMR Spectrum of 6al.**

**ESI-MASS Spectrum of 6al.**
$^1$H NMR Spectrum of 6am.

$^{13}$C NMR Spectrum of 6am.
$^1$H NMR Spectrum of 6an.

$^{13}$C NMR Spectrum of 6an.
$^{1}$H NMR Spectrum of 6ao.

$^{13}$C NMR Spectrum of 6ao.
$^1$H NMR Spectrum of 6ap.

$^{13}$C NMR Spectrum of 6ap.
$^1$H NMR Spectrum of 6aq.

$^{13}$C NMR Spectrum of 6aq.
DEPT-135 NMR Spectrum of 6aq.

$^1$H NMR Spectrum of 6ar.
$^{13}$C NMR Spectrum of 6ar.

$^1$H NMR Spectrum of 6as.
\(^{13}\)C NMR Spectrum of 6as.

\(^{1}\)H NMR Spectrum of 6at.
$^{13}$C NMR Spectrum of 6at.

DEPT-135 NMR Spectrum of 6at.
$^1$H NMR Spectrum of 6au.

$^{13}$C NMR Spectrum of 6au
1. **Data Collection**

A Leica MZ 7s microscope was used to identify a suitable colorless block with very well defined faces with dimensions (max, intermediate, and min) 0.08 x 0.02 x 0.02 mm$^3$ from a representative sample of crystals of the same habit. The crystal mounted on a nylon loop was then placed in a cold nitrogen stream (Oxford) maintained at 110 K.

A BRUKER GADDS X-ray (three-circle) diffractometer was employed for crystal screening, unit cell determination, and data collection. The goniometer was controlled using the FRAMBO software, v.4.1.05.\(^1\) The sample was optically centered with the aid of a video camera such that no translations were observed as the crystal was rotated through all positions. The detector was set at 5.0 cm from the crystal sample. The X-ray radiation employed was generated from a Cu sealed X-ray tube (K$_\alpha$ = 1.5418 Å with a potential of 40 kV and a current of 40 mA) fitted with a graphite monochromator in the parallel mode (175 mm collimator with 0.5 mm pinholes).

180 data frames were taken at widths of 0.5°. These reflections were used to determine the unit cell using Cell_Now.\(^2\) The unit cell was verified by examination of the $h \ k \ l$ overlays on several frames of data. No super-cell or erroneous reflections were observed.

After careful examination of the unit cell, an extended data collection procedure (11 sets) was initiated using omega and phi scans.

**Data Reduction, Structure Solution, and Refinement**

Integrated intensity information for each reflection was obtained by reduction of the data frames with APEX2.\(^3\) The integration method employed a three dimensional profiling algorithm and all data were corrected for Lorentz and polarization factors, as well as for crystal decay effects. Finally the data was merged and scaled to produce a suitable data set. SADABS\(^4\) was employed to correct the data for absorption effects.

Systematic reflection conditions and statistical tests indicated the space group $C2/c$. A solution was obtained readily using XT/ XS.\(^3\)\(^5\) Hydrogen atoms were placed in idealized positions and were refined
using riding model. All non-hydrogen atoms were refined with anisotropic thermal parameters. The structure was refined (weighted least squares refinement on $F^2$) to convergence.\textsuperscript{5,6} Platon\textsuperscript{*} was used to verify the absence of additional symmetry. Platon,\textsuperscript{*} though, indicated presence of voids of volume 517.4 Å$^3$, corresponding to 23 e$^-$ per unit cell; the residual electron density map did not indicate any possible solvents. Upon SQUEEZE, the reliability factor did not decrease significantly indicating no possible contents in the voids.

OLEX2 was employed for the structure plots.\textsuperscript{6}

\begin{flushleft}
\textsuperscript{1} FRAMBO v. 4.1.05 “Program for Data Collection on Area Detectors” BRUKER-Nonius Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA
\textsuperscript{2} Sheldrick, G. M. “Cell_NOW (version 2008/1): Program for Obtaining Unit Cell Constants from Single Crystal Data”: University of Göttingen, Germany
\textsuperscript{3} APEX2 “Program for Data Collection and Integration on Area Detectors” BRUKER AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA
\textsuperscript{4} Sheldrick, G.M. “SADABS: Program for Absorption Correction for Data from Area Detector Frames”, University of Göttingen.
\end{flushleft}
| **Table 1. Crystal data and structure refinement for PTB_150921_G_5AM.** |
|-------------------------------------|-----------------|
| **Identification code**            | psa5am          |
| **Empirical formula**              | C27 H20 Cl N3 O3 |
| **Formula weight**                 | 469.91          |
| **Temperature**                    | 110.0 K         |
| **Wavelength**                     | 1.54178 Å       |
| **Crystal system**                 | Monoclinic      |
| **Space group**                    | C 1 2/c 1       |
| **Unit cell dimensions**           |                 |
| a = 29.0413(17) Å                  | α = 90°         |
| b = 12.5389(6) Å                   | β = 92.096(4)°  |
| c = 13.3299(6) Å                   | γ = 90°         |
| **Volume**                         | 4850.8(4) Å³    |
| **Z**                              | 8               |
| **Density (calculated)**           | 1.287 Mg/m³     |
| **Absorption coefficient**         | 1.668 mm⁻¹      |
| **F(000)**                         | 1952            |
| **Crystal size**                   | 0.08 x 0.02 x 0.02 mm³ |
| **Theta range for data collection**| 3.045 to 60.568° |
| **Index ranges**                   | -32<=h<=32, -13<=k<=13, -15<=l<=15 |
| **Reflections collected**          | 25107           |
| **Independent reflections**        | 3533 [R(int) = 0.0525] |
| **Completeness to theta = 67.679°**| 80.7 %         |
| **Absorption correction**          | Semi-empirical from equivalents |
| **Max. and min. transmission**     | 0.7519 and 0.6553 |
| **Refinement method**              | Full-matrix least-squares on F² |
| **Data / restraints / parameters** | 3533 / 0 / 308 |
| **Goodness-of-fit on F²**           | 1.096           |
| **Final R indices [I>2sigma(I)]**  | R1 = 0.0343, wR2 = 0.0853 |
| **R indices (all data)**           | R1 = 0.0427, wR2 = 0.0888 |
| **Extinction coefficient**         | n/a             |
| **Largest diff. peak and hole**    | 0.213 and -0.342 e.Å⁻³ |