Supporting Information

Cu-Catalyzed C-H Amination/Ullmann N-Arylation Domino Reaction: Straightforward Synthesis of 9,14-Diaryl-9,14-dihydrodibenzo[a,c]phenazine

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I. General Information

Unless otherwise noted, all reagents were obtained commercially available and used without further purification.

NMR spectrum: $^1$H and $^{13}$C NMR spectra were collected on 400 MHz and 300 MHz NMR spectrometers (Bruker AVANCE) using CDCl$_3$ or DMSO-d$_6$. Chemical shifts are reported in parts per million (ppm). Chemical shifts for protons are reported in parts per million downfield and are referenced to residual protium in the NMR solvent (CHCl$_3$ = $\delta$ 7.26). Chemical shifts for carbon are reported in parts per million downfield and are referenced to the carbon resonances of the solvent (CDCl$_3$ = $\delta$ 77.0). Data are represented as follows: chemical shift, multiplicity (br. s = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz), integration.

Mass spectroscopy: Mass spectra were in general recorded on an AMD 402/3 or a HP 5989A mass selective detector.

Column Chromatography: Column chromatography was performed with silica gel (200-300 mesh ASTM).
II. The Data and NMR Spectra of Products

11-methyl-9,14-diphenyl-9,14-dihydrodibenzo[a,c]phenazine (1aa)
m.p. 183-185 °C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$: 8.68 (d, $J = 8.0$ Hz, 2H), 8.07-8.12 (m, 2H), 7.68-7.73 (m, 2H), 7.46-7.61 (m, 4H), 7.21-7.29 (m, 2H), 6.92-7.03 (m, 6H), 6.75-6.82 (m, 3H), 2.12 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$: 148.04, 145.42, 145.31, 144.20, 138.30, 137.47, 131.02, 130.01, 129.79, 129.57, 129.47, 128.82, 127.45, 127.02, 126.89, 126.70, 126.44, 126.39, 125.49, 125.02, 124.68, 124.57, 123.03, 120.85, 118.14, 116.50, 20.52; HRMS ESI (m/z) [M]$^+$: calcd. for C$_{33}$H$_{24}$N$_2$ 448.1939, found 448.1938.
11-methoxy-9,14-diphenyl-9,14-dihydrodibenzo[a,c]phenazine (1ab)
m.p. 138-140 °C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$: 8.71 (d, $J = 8.4$ Hz, 2H), 8.15 (d, $J = 8.0$ Hz, 1H), 8.09 (d, $J = 8.4$ Hz, 1H), 7.67-7.71 (m, 2H), 7.54-7.65 (m, 3H), 7.47-7.52 (m, 1H), 7.28-7.31 (m, 2H), 7.03-7.06 (m, 4H), 6.94 (d, $J = 8.0$ Hz, 2H), 6.79-6.82 (m, 1H), 6.60-6.62 (m, 2H), 3.66 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$: 155.18, 148.44, 145.78, 143.38, 141.53, 138.44, 136.62, 130.07, 129.58, 129.55, 129.28, 128.74, 127.53, 127.00, 126.72, 126.29, 126.18, 125.62, 125.56, 124.62, 124.51, 124.39, 122.95, 122.89, 121.39, 120.62, 116.08, 114.16, 55.36; HRMS ESI ($m/z$) [M]$^+$: calcd. for C$_{33}$H$_{24}$N$_2$O 464.1889, found 464.1890.
methyl 4-(14-phenyldibenzo[a,c]phenazin-9(14H)-yl)benzoate (1ac)
m.p. 182-185 °C; 1H NMR (400 MHz, CDCl$_3$) $\delta$: 8.74-8.77 (m, 2H), 8.09-8.11 (m, 1H), 8.03-8.06 (m, 1H), 7.79-7.82 (m, 1H), 7.73-7.75 (m, 1H), 7.65-7.70 (m, 4H), 7.52-7.60 (m, 2H), 7.37-7.40 (m, 2H), 6.96-7.03 (m, 4H), 6.89-6.91 (m, 2H), 6.77-6.81 (m, 1H), 3.78 (s, 3H); 13C NMR (100 MHz, CDCl$_3$) $\delta$: 166.94, 151.03, 147.07, 145.26, 143.49, 138.87, 137.13, 130.71, 130.11, 129.79, 129.22, 128.94, 128.87, 127.77, 127.46, 127.21, 127.07, 126.90, 126.77, 126.12, 125.39, 124.76, 124.24, 123.19, 123.09, 121.59, 121.48, 116.99, 114.18, 51.65; HRMS ESI (m/z) [M]$^+$: calcd. for C$_{34}$H$_{24}$N$_2$O$_2$ 492.1838, found 492.1836.
9,14-diphenyl-9,14-dihydrodibenzo[a,c]phenazine (1ad)
m.p. 241-243 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 8.74 (d, \(J = 8.0\) Hz, 2H), 8.12 (d, \(J = 8.0\) Hz, 2H), 7.74-7.76 (m, 2H), 7.63-7.67 (m, 2H), 7.52-7.56 (m, 2H), 7.33-7.35 (m, 2H), 6.96-7.04 (m, 8H), 6.76-6.80 (m, 2H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\): 147.69, 144.83, 138.13, 129.88, 129.48, 128.76, 127.39, 126.98, 126.51, 125.37, 124.61, 123.02, 121.02, 116.76; HRMS ESI (m/z) [M+H]\(^+\): calcd. for C\(_{32}\)H\(_{23}\)N\(_2\) 435.1861, found 435.1851.
9-(4-bromophenyl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ae)

m.p. 188-189 °C; \(^1\)H NMR (400 MHz, DMSO) \(\delta\): 8.95 (d, \(J = 8.4\) Hz, 2H), 8.02-7.86 (m, 4H), 7.78-7.58 (m,4H), 7.50-7.39 (m, 2H), 7.22 (d, \(J = 9.1\) Hz,2H), 7.14-7.05 (m, 2H), 7.01 (d, \(J = 7.8\) Hz, 2H), 6.91-6.81 (m, 3H); \(^{13}\)C NMR (100 MHz, CDCl3) \(\delta\) 147.35, 146.69, 144.95, 144.22, 138.43, 137.50, 131.49, 129.94, 129.84, 129.29, 129.06, 128.84, 127.43, 127.10, 127.03, 126.70, 126.64, 125.72, 125.41, 124.65, 124.26, 123.11, 123.02, 121.25, 117.68, 116.71, 113.13; HRMS ESI (m/z) [M+H]\(^+\): calcd. for C\(_{32}\)H\(_{22}\)N\(_2\)Br 513.0966, found 513.0968.
4-(14-phenyldibenzo[a,c]phenazin-9(14H)-yl)benzonitrile (1ae)

m.p. 231-231 °C; $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$: 8.97-9.00 (m, 2H), 8.02-8.04 (m, 1H), 7.93-7.97 (m, 3H), 7.69-7.80 (m, 3H), 7.61-7.65 (m, 1H), 7.48-7.52 (m, 4H), 7.08-7.11 (m, 2H), 7.02-7.04 (m, 2H), 6.93-6.96 (m, 2H), 6.84-6.88 (m, 1H); $^{13}$C NMR (100 MHz, CDCl3) $\delta$: 150.76, 146.89, 145.35, 142.97, 139.15, 136.64, 133.09, 130.19, 129.81, 129.11, 128.95, 128.68, 127.74, 127.64, 127.44, 127.22, 127.17, 126.97, 126.56, 125.56, 124.85, 123.91, 123.36, 123.16, 121.73, 119.72, 117.00, 114.73, 102.52.; HRMS ESI (m/z) [M+H]$^+$: calcd. for C$_{33}$H$_{22}$N$_3$ 460.1814, found 460.1813.
9-(naphthalen-1-yl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ag)
m.p. 215-218 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.66-8.70 (m, 2H), 8.61-8.63 (d, \(J = 8.4\) Hz, 1H), 8.32-8.35 (m, 1H), 7.88-7.91 (m, 2H), 7.74-7.76 (d, \(J = 8.0\) Hz, 1H), 7.61-7.64 (m, 3H), 7.43-7.56 (m, 4H), 7.17-7.26 (m, 3H), 7.03-7.14 (m, 4H), 6.87-6.91 (m, 3H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 150.28, 146.61, 143.84, 139.38, 138.30, 135.07, 132.53, 131.41, 130.29, 130.15, 128.94, 128.62, 127.96, 127.88, 127.35, 127.21, 126.69, 126.29, 126.06, 125.90, 125.78, 125.30, 124.20, 123.87, 123.48, 123.12, 122.78, 120.28, 120.11, 115.14; HRMS ESI (\(m/z\)) [M+H]\(^+\): calcld. for C\(_{36}\)H\(_{25}\)N\(_2\) 485.2018, found 485.2011.
9-(phenanthren-9-yl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ah)
m.p. 282-285 °C; \( ^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \): 8.96-8.98 (m, 1H), 8.76-8.78 (m, 1H), 8.69-8.71 (d, \( J =8.4 \) Hz, 2H), 8.61-8.63 (d, \( J =8.4 \) Hz, 1H), 8.40-8.42(m, 1H), 8.09-8.11 (d, \( J =8.4 \) Hz, 1H), 7.74-7.79 (m, 2H), 7.52-7.67 (m, 5H), 7.33-7.48 (m, 3H), 7.03-7.22 (m, 6H), 6.92-7.00 (m, 3H); \( ^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \): 150.90, 147.07, 142.91, 140.10, 139.42, 132.94, 132.02, 131.85, 131.51, 130.23, 129.60, 128.99, 128.57, 128.15, 127.59, 127.39, 127.10, 126.94, 126.82, 126.38, 125.99, 124.24, 123.89, 123.36, 123.09, 122.83, 122.35, 120.86, 120.36, 115.33; HRMS ESI (\( m/z \)) [M+H]+: calcd. for C\(_{40}\)H\(_{27}\)N\(_2\) 535.2174, found 535.2175.
9-phenyl-14-(pyren-1-yl)-9,14-dihydrodibenz[a,c]phenazine (1ai)

m.p. 324-326 °C; $^1$H NMR (400 MHZ, CDCl$_3$) $\delta$: 8.89-8.91 (d, $J=9.2$ Hz, 1H), 8.68-8.70 (d, $J=8.0$ Hz, 2H), 8.38-8.40 (m, 1H), 8.22-8.26 (t, $J=8.0$ Hz, 2H), 8.17-8.19 (d, $J=8.4$ Hz, 1H), 8.04-8.08 (m, 2H), 7.93-7.97 (m, 2H), 7.85-7.87 (d, $J=8.0$ Hz, 1H), 7.64-7.66 (m, 4H), 7.57-7.59 (d, $J=8.0$ Hz, 1H), 7.39-7.43 (t, $J=7.6$ Hz, 1H), 7.15-7.21 (m, 3H), 6.92-7.01 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$: 150.43, 146.93, 141.34, 139.21, 138.40, 131.82, 131.26, 131.01, 130.45, 130.31, 130.15, 129.62, 129.07, 128.97, 128.79, 128.38, 127.96, 127.67, 127.36, 127.27, 127.18, 126.40, 126.35, 125.95, 125.91, 125.83, 125.81, 125.76, 125.46, 124.76, 124.48, 124.26, 123.92, 123.50, 123.09, 122.79, 120.37, 120.25, 115.26; HRMS ESI (m/z) [M]$^+$: calcd. for C$_{42}$H$_{26}$N$_2$: 558.2096, found 558.2095.
9-(9,9-dimethyl-9H-fluoren-2-yl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1aj)

m.p. 226-228 °C; ^1H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\): 8.95 (d, \(J = 8.0 \text{ Hz}\), 2H), 7.99-8.05 (m, 3H), 7.87-7.90 (m, 1H), 7.55-7.75 (m, 6H), 7.37-7.45 (m, 3H), 7.16-7.26 (m, 3H), 7.06-7.10 (m, 3H), 6.98-7.01 (d, \(J = 8.0 \text{ Hz}\), 2H), 6.80 (t, \(J = 7.2 \text{ Hz}\), 1H), 1.10 (s, 6H); ^13C NMR (100 MHz, CDCl\(_3\)) \(\delta\): 154.63, 153.32, 148.16, 147.59, 145.60, 144.58, 139.03, 138.71, 137.89, 132.96, 129.96, 129.84, 129.66, 129.45, 128.75, 127.70, 127.07, 126.86, 126.80, 126.52, 126.47, 126.10, 125.60, 125.22, 124.62, 124.57, 123.00, 122.31, 120.85, 120.20, 119.17, 117.24, 116.34, 112.70, 46.61, 26.89; HRMS ESI (m/z) [M]+: calcd. for C\(_{41}\)H\(_{30}\)N\(_2\) 550.2409, found 550.2407.
11-methyl-14-phenyl-9-(p-tolyl)-9,14-dihydrodibenzo[a,c]phenazine (1dd)

m.p. 254-255 °C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$: 8.71 (d, $J = 8.3$ Hz, 2H), 8.06-8.15 (m, 2H), 7.47-7.64 (m, 6H), 7.10 (dd, $J = 8.0, 1.1$ Hz, 1H), 7.01 (dd, $J = 11.3, 4.6$ Hz, 2H), 6.89-6.96 (m, 4H), 6.82 (d, $J = 8.4$ Hz, 2H), 6.77 (dd, $J = 12.2, 5.0$ Hz, 1H), 2.44 (s, 3H), 2.14 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$: 148.25, 145.40, 145.16, 141.53, 138.40, 137.64, 135.37, 130.93, 129.96, 129.70, 129.60, 129.48, 129.40, 128.71, 127.14, 126.96, 126.82, 126.35, 126.30, 125.61, 124.62, 124.58, 122.98, 122.95, 120.50, 118.21, 116.19, 21.34, 20.49; HRMS ESI (m/z) [M]$^+$: calcd. for C$_{34}$H$_{26}$N$_2$ 462.2096, found 462.2090.
11-methoxy-9-(4-methoxyphenyl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ed)
m.p. 226-228 °C; $^1$H NMR (400 MHz, DMSO) δ: 8.91 (d, $J = 8.3$ Hz, 2H), 7.99 (dd, $J = 16.5$, 8.0 Hz, 2H), 7.61-7.72 (m, 4H), 7.54 (t, $J = 7.6$ Hz, 1H), 7.41 (s, 1H), 7.16 (d, $J = 8.9$ Hz, 2H), 7.09 (t, $J = 7.8$ Hz, 2H), 6.93 (d, $J = 8.8$ Hz, 1H), 6.87 (d, $J = 8.1$ Hz, 2H), 6.81 (t, $J = 7.3$ Hz, 1H), 6.70 (d, $J = 8.9$ Hz, 2H), 3.85 (s, 3H), 3.61 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 157.63, 155.45, 149.22, 146.97, 141.34, 138.53, 136.93, 136.28, 130.12, 129.73, 129.51, 129.27, 128.71, 128.06, 127.08, 126.71, 126.29, 126.23, 124.53, 124.48, 123.01, 122.90, 122.06, 120.31, 115.77, 114.24, 111.22, 109.68, 55.77, 55.40; HRMS ESI (m/z) [M+H]+: calcd. for C$_{34}$H$_{27}$N$_2$O$_4$ 495.2073, found 495.2075.
methyl 9-(4-(methoxycarbonyl)phenyl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine-11-carboxylate (1fd)

m.p. 271-272 °C; \(^1\)H NMR (400 MHz, DMSO) \(\delta\): 8.97 (d, \(J = 8.3\) Hz, 2H), 8.40 (d, \(J = 1.9\) Hz, 1H), 8.15 (d, \(J = 8.4\) Hz, 1H), 8.03-8.08 (m, 2H), 7.89-7.94 (m, 1H), 7.72-7.76 (m, 2H), 7.67-7.71 (m, 3H), 7.57-7.60 (t, \(J = 7.6\) Hz, 1H), 7.13-7.20 (m, 4H), 6.89-6.97 (m, 3H), 3.92 (s, 3H), 3.72 (s, 3H); \(^13\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\): 166.88, 166.31, 151.13, 149.83, 146.36, 142.61, 137.98, 136.12, 130.86, 130.34, 129.84, 129.20, 128.95, 128.75, 128.74, 127.84, 127.43, 127.06, 127.02, 126.99, 126.94, 125.96, 124.64, 124.16, 123.20, 122.83, 122.18, 118.76, 114.40, 52.44, 51.74; HRMS ESI (m/z) [M+H]\(^+\): calcd. for C\(_{36}\)H\(_{27}\)N\(_2\)O\(_4\) 551.1971, found 551.1970.
11-methyl-9,14-diphenyl-9,14-dihydrophenanthro[4,5-abc]phenazine (1ca)

m.p. 221-224 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ: 8.36 (dd, $J = 15.9$, 7.7 Hz, 2H), 8.16 (t, $J = 6.8$ Hz, 2H), 8.09 (s, 2H), 8.01-7.86 (m, 2H), 7.85-7.67 (m, 2H), 7.39-7.28 (m, 2H), 7.13-6.96 (m, 6H), 6.92-6.75 (m, 3H), 2.17 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 148.19, 145.46, 145.16, 143.94, 138.84, 137.88, 131.31, 131.28, 129.43, 128.75, 128.35, 128.23, 127.38, 127.34, 127.21, 126.27, 126.07, 125.93, 125.41, 125.10, 125.00, 124.88, 123.98, 123.73, 121.86, 121.69, 120.96, 118.76, 116.90, 20.45; HRMS ESI (m/z) [M+H]$^+$: calcd. for C$_{35}$H$_{28}$N$_2$ 473.2018, found 473.2021.
9,14-diphenyl-9,14-dihydrophenanthro[4,5-abc]phenazine (1cc)

m.p. 240-241 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ: 8.37 (d, $J = 7.8$ Hz, 2H), 8.18 (d, $J = 7.5$ Hz, 2H), 8.10 (s, 2H), 7.94 (t, $J = 7.8$ Hz, 2H), 7.86-7.74 (m, 2H), 7.36 (dd, $J = 5.9$, 3.4 Hz, 2H), 7.12-6.98 (m, 8H), 6.81 (t, $J = 6.8$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ: 147.90, 144.75, 138.77, 131.44, 128.81, 128.38, 127.47, 127.18, 126.13, 125.37, 125.25, 123.95, 121.87, 121.29, 117.35; HRMS ESI (m/z) [M+H]$^+$: calcd. for C$_{34}$H$_{23}$N$_2$ 459.1861, found 459.1861.
dimethyl 4,4'-dibenzo[a,c]phenazine-9,14-diyl)dibenzoate (1cc-2)

$^1$H NMR (400 MHz, DMSO) $\delta$: 9.01 (d, $J = 8.3$ Hz, 2H), 8.02 (dt, $J = 7.3$, 3.7 Hz, 2H), 7.94-7.98 (m, 2H), 7.77-7.82 (m, 2H), 7.69 (t, $J = 7.4$ Hz, 2H), 7.64 (d, $J = 9.0$ Hz, 4H), 7.54 (dd, $J = 5.9$, 3.4 Hz, 2H), 6.97 (d, $J = 9.0$ Hz, 4H), 3.70 (s, 6H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 166.83, 150.43, 144.06, 138.06, 130.85, 130.05, 128.76, 128.08, 127.38, 127.26, 126.27, 124.47, 123.32, 122.04, 114.25, 51.74; HRMS ESI (m/z) [M+H]+: calcd. for C$_{36}$H$_{27}$N$_2$O$_4$ 551.1971, found 551.1840.
9-methyl-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (4)

m.p. 212-213 °C; $^1$H NMR (400 MHz, DMSO) $\delta$: 8.91 (dd, $J = 6.8$, 2.7 Hz, 1H), 8.82 (d, $J = 7.7$ Hz, 1H), 8.26-8.31 (m, 1H), 7.96 (dd, $J = 8.0$, 1.3 Hz, 1H), 7.74 (m, 2H), 7.67 (dd, $J = 7.8$, 1.3 Hz, 1H), 7.50-7.60 (m, 2H), 7.35 (dd, $J = 7.9$, 1.3 Hz, 1H), 7.26 (m, 1H), 7.13-7.19 (m, 3H), 7.04 (d, $J = 7.8$ Hz, 2H), 6.93 (t, $J = 7.2$ Hz, 1H), 3.53 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$: 150.58, 141.65, 139.64, 133.55, 130.44, 129.42, 128.79, 127.29, 127.03, 126.82, 126.40, 126.04, 125.48, 123.95, 123.79, 123.34, 123.09, 122.74, 121.23, 117.55, 116.67, 43.71; HRMS ESI (m/z) [M+H]$^+$: calcd. for C$_{37}$H$_{20}$N$_2$ 373.1705, found 373.1691.
III. The X-ray Analysis

Identification code 

Empirical formula C33 H24 N2

Formula weight 448.54

Temperature 293(2) K

Wavelength 0.71073 Å

Crystal system Monoclinic

Space group P 21/n

Unit cell dimensions 

\[ a = 13.670(2) \text{ Å} \]
\[ b = 10.7087(18) \text{ Å} \]
\[ c = 16.477(3) \text{ Å} \]

\[ \alpha = 90^\circ. \]
\[ \beta = 98.766(4)^\circ. \]

\[ \gamma = 90^\circ. \]

Volume 2384.0(7) Å

Z

4

Density (calculated) 1.250 Mg/m³

Absorption coefficient 0.073 mm⁻¹

F(000) 944

Crystal size 0.220 x 0.170 x 0.130 mm³

Theta range for data collection 1.806 to 25.500°.

Index ranges -15<=h<=16, -11<=k<=12, -19<=l<=19

Reflections collected 13421

Independent reflections 4424 [R(int) = 0.0480]

Completeness to theta = 25.242° 100.0 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7456 and 0.6237

Refinement method Full-matrix least-squares on F²

Data / restraints / parameters 4424 / 0 / 317
Goodness-of-fit on $F^2$ 1.095

Final R indices [I>2sigma(I)] R1 = 0.0653, wR2 = 0.1363

R indices (all data) R1 = 0.1028, wR2 = 0.1521

Extinction coefficient n/a

Largest diff. peak and hole 0.264 and -0.160 e.Å$^{-3}$

Identification code cd21251

Empirical formula C34.50 H25 Cl N2 O2

Formula weight 535.02

Temperature 293(2) K

Wavelength 0.71073 Å

Crystal system, space group Monoclinic, C2/c

Unit cell dimensions
\[
\begin{align*}
a &= 15.3088(9) \text{ Å} & \alpha &= 90 \text{ deg.} \\
b &= 17.9930(11) \text{ Å} & \beta &= 92.570(2) \text{ deg.} \\
c &= 19.4932(12) \text{ Å} & \gamma &= 90 \text{ deg.}
\end{align*}
\]

Volume 5364.0(6) Å$^3$

Z, Calculated density 8, 1.325 Mg/m$^3$

Absorption coefficient 0.178 mm$^{-1}$

F(000) 2232

Crystal size 0.311 x 0.257 x 0.205 mm

Theta range for data collection 1.75 to 25.50 deg.

Limiting indices h=-18<=h<=18, k=-20<=k<=21, l=-23<=l<=23

Reflections collected / unique 15604 / 5002 [R(int) = 0.0233]

Completeness to theta = 25.50 99.9 %

Absorption correction Empirical

Max. and min. transmission 1.00000 and 0.77314

Refinement method Full-matrix least-squares on $F^2$

Data / restraints / parameters 5002 / 0 / 358
Goodness-of-fit on \( F^2 \)  
\[ 1.019 \]

Final R indices \([I>2\sigma(I)]\)  
\[ R1 = 0.0581, \ wR2 = 0.1653 \]

R indices (all data)  
\[ R1 = 0.0710, \ wR2 = 0.1780 \]

Largest diff. peak and hole  
\[ 0.491 \text{ and } -0.650 \text{ e.A}^{-3} \]

Identification code  
\[ \text{cd211425} \]

Empirical formula  
\[ \text{C}_{36} \text{H}_{24} \text{N}_{2} \]

Formula weight  
\[ 484.57 \]

Temperature  
\[ 293(2) \text{ K} \]

Wavelength  
\[ 0.71073 \text{ A} \]

Crystal system, space group  
\[ \text{Monoclinic, C2/c} \]

Unit cell dimensions  
\[ a = 14.0547(18) \text{ A} \quad \alpha = 90 \text{ deg.} \]
\[ b = 19.251(3) \text{ A} \quad \beta = 90.832(3) \text{ deg.} \]
\[ c = 18.410(2) \text{ A} \quad \gamma = 90 \text{ deg.} \]

Volume  
\[ 4980.7(11) \text{ A}^3 \]

Z, Calculated density  
\[ 8, 1.292 \text{ Mg/m}^3 \]

Absorption  
\[ 0.075 \text{ mm}^{-1} \]

\( F(000) \)  
\[ 2032 \]

Crystal size  
\[ 0.309 \times 0.238 \times 0.197 \text{ mm} \]

Theta range for data collection  
\[ 2.10 \text{ to } 26.00 \text{ deg.} \]

Limiting indices  
\[ -17 \leq h \leq 16, \ -23 \leq k \leq 23, \ -22 \leq l \leq 12 \]

Reflections collected / unique  
\[ 13435 / 4891 \quad [R(int) = 0.0210] \]

Completeness to theta = 26.00  
\[ 99.8 \% \]

Absorption correction  
\[ \text{Empirical} \]

Max. and min.  
\[ 1.00000 \text{ and } 0.84202 \]

Refinement method  
\[ \text{Full-matrix least-squares on } F^2 \]

Data / restraints / parameters  
\[ 4891 / 0 / 343 \]

Final R indices \([I>2\sigma(I)]\)  
\[ R1 = 0.0398, \ wR2 = 0.1038 \]

R indices (all data)  
\[ R1 = 0.0549, \ wR2 = 0.1145 \]

Largest diff. peak and hole  
\[ 0.181 \text{ and } -0.145 \text{ e.A}^{-3} \]

\[ 1ag \]
Identification code                 cd21252
Empirical formula                 C42 H26 N2
Formula weight                    558.65
Temperature                       293(2) K
Wavelength                       0.71073 Å
Crystal system, space group          Monoclinic,  P2(1)/n
Unit cell dimensions                 a = 11.4684(6) Å   alpha = 90 deg.
                                                                      b = 18.0050(9) Å    beta = 92.9890(10) deg.
                                                                      c = 13.8450(7) Å   gamma = 90 deg.
Volume                            2854.9(3) Å³
Z, Calculated density                4, 1.300 Mg/m³
Absorption coefficient                0.075 mm⁻¹
F(000)                            1168
Crystal size                        0.321 x 0.212 x 0.156 mm
Theta range for data collection         1.86 to 26.00 deg.
Limiting indices                    -14<=h<=13, -22<=k<=16, -17<=l<=17
Reflections collected / unique         17144 / 5607 [R(int) = 0.0235]
Completeness to theta = 26.00          99.9 %
Absorption correction                Empirical
Max. and min. transmission           1.00000 and 0.58903
Refinement method                  Full-matrix least-squares on F²
Data / restraints / parameters           5607 / 6 / 397
Goodness-of-fit on F²                1.023
Final R indices [I>2sigma(I)]         R1 = 0.0486, wR2 = 0.1257
R indices (all data)                 R1 = 0.0703, wR2 = 0.1407
Largest diff. peak and hole          0.163 and -0.122 e.A⁻³