SUPPLEMENTARY DATA

DABCO CATALYSED MULTICOMPONENT REACTION FOR SYNTHESIS OF BENZO[*a*]CARBAZOLES

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The same experimental procedure is repeated for the synthesis the following compounds using 4-bromobenzaldehyde, *N,N* dimethylaminobenzaldehyde, pyridine-3-aldehyde, 5-bromothiophene-2-carbaldehyde.

2-Amino-4-(4'-bromo-phenyl)-8-methyl-5,6-dihydro-11H-benzo[*a*]carbazole-1,3-dicarbonitrile (5a)

Yellow solid; yield: 81%; m.p. 231-233 °C; IR (KBr, cm⁻¹)_v_{max}: 3452 (asym, NH₂), 3317 (sym, NH₂), 2231 (C≡N); ¹H NMR (500 MHz, CDCl₃) (ppm) δ_H: 8.89 (b s, 1H, N₁₁-H), 7.56-7.46 (m, 3H, C₇, C₉ & C₁₀ -H), 7.39-7.36 (m, 4H, C₂', C₃', C₅' & C₆'-H), 5.11 (s, 2H, NH₂), 2.95 (m, 2H, C₅-2H), 2.84 (m, 2H, C₆-2H), 2.67 (s, 3H, C₈-CH₃); ¹³C NMR (125 MHz, CDCl₃) (ppm) δ_C: 154.4 (C₂), 146.3 (C_{11b}), 145.1 (C₄), 137.0 (C_{10a}), 131.6 (C₁'), 130.9 (C₂' & C₆'), 129.1 (C_{4a}), 128.2 (C₈), 126.4 (C_{6b}), 125.1 (C₄'), 124.3 (C₃' & C₅'), 122.3 (C_{11a}), 121.2 (C₉), 119.9 (C₇), 117.1 (C_{6a}), 115.8 (C≡N), 114.1 (C≡N), 111.3 (C₁₀), 94.1 (C₃), 93.9 (C₁), 29.0 (C₅), 23.7 (C₆), 21.6 (C₈-CH₃); MS: m/z (%) 453 (M⁺ 100), 455 (M+2); Anal.Calcd.for C₂₅H₁₇BrN₄: C, 66.24; H, 3.78; N, 12.36. Found : C, 66.21; H, 3.75; N, 12.34 %

2-Amino-4-(4'-dimethylamino-phenyl)-8-methyl-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (6a)

Yellow solid; yield: 80%; m.p. 235-237 °C; IR (KBr, cm^{-1}) ν_{max} : 3432 (asym, NH_2), 3327 (sym, NH_2), 2215 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.90 (b s, 1H, $\text{N}_{11}\text{-H}$), 7.58-7.47 (m, 3H, C_7 , C_9 & C_{10} -H), 7.45-7.30 (m, 4H, C_2' , C_3' , C_5' & C_6' -H), 5.40 (s, 2H, NH_2), 3.27 (s, 6H, $\text{N}(\text{CH}_3)_2$), 2.98 (m, 2H, $\text{C}_5\text{-2H}$), 2.80 (m, 2H, $\text{C}_6\text{-2H}$), 2.55 (s, 3H, $\text{C}_8\text{-CH}_3$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 155.6 (C_4'), 151.7 (C_2), 147.0 ($\text{C}_{11\text{b}}$), 145.5 (C_4), 136.4 ($\text{C}_{10\text{a}}$), 130.4 (C_2' & C_6'), 129.1 ($\text{C}_{4\text{a}}$), 128.9 (C_8), 127.0 ($\text{C}_{6\text{b}}$), 123.1 (C_1'), 122.7 ($\text{C}_{11\text{a}}$), 122.0 (C_9), 118.3 (C_7), 117.7 ($\text{C}_{6\text{a}}$), 115.9 ($\text{C}\equiv\text{N}$), 114.7 ($\text{C}\equiv\text{N}$), 113.3 (C_3' & C_5'), 110.4 (C_{10}), 96.0 (C_3), 94.2 (C_1), 43.1 ($\text{N}(\text{CH}_3)_2$), 29.6 (C_5), 24.2 (C_6), 21.9 ($\text{C}_8\text{-CH}_3$); MS: m/z (%) 453 (M^+ 100); Anal.Calcd.for $\text{C}_{27}\text{H}_{23}\text{N}_5$: C, 77.67; H, 5.55; N, 16.77. Found: C, 77.68; H, 5.53; N, 16.74 %

2-Amino-4-(pyridin-3'-yl)-8-methyl-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (7a)

Yellow solid; yield: 82%; m.p. 232-234 °C; IR (KBr, cm^{-1}) ν_{max} : 3451 (asym, NH_2), 3348 (sym, NH_2), 2241 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 9.33 (s, 1H, $\text{N}_{11}\text{-H}$), 7.71-7.66 (m, 4H, C_2' , C_4' , C_5' & C_6' -H), 7.58- 7.41 (m, 3H, C_7 , C_9 & C_{10} -H), 5.39 (s, 2H, NH_2), 2.87 (m, 2H, $\text{C}_5\text{-2H}$), 2.67 (m, 2H, $\text{C}_6\text{-2H}$), 2.59 (s, 3H, $\text{C}_8\text{-CH}_3$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 153.2 (C_2), 150.3 (C_2'), 149.6 (C_4'), 148.1 ($\text{C}_{11\text{b}}$), 145.7 (C_4), 138.1 (C_6'), 137.1 ($\text{C}_{10\text{a}}$), 135.2 (C_1'), 130.2 ($\text{C}_{4\text{a}}$), 129.1 (C_8), 128.5 ($\text{C}_{6\text{b}}$), 126.8 (C_5'), 123.1 ($\text{C}_{11\text{a}}$), 122.8 (C_9), 119.6 (C_7), 118.6 ($\text{C}_{6\text{a}}$), 115.6 ($\text{C}\equiv\text{N}$), 114.5 ($\text{C}\equiv\text{N}$), 111.2 (C_{10}), 96.6 (C_3), 95.1 (C_1), 30.0 (C_5), 24.9 (C_6), 21.6 ($\text{C}_8\text{-CH}_3$); MS: m/z (%) 375 (M^+ 100); Anal.Calcd.for $\text{C}_{24}\text{H}_{17}\text{N}_5$: C, 76.78; H, 4.58; N, 18.65. Found: C, 76.76; H, 4.56; N, 18.63 %

2-Amino-4-(5'-bromothiophen-2'-yl)-8-methyl-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (8a)

Yellow solid; yield: 80%; m.p. 240-242 °C; IR (KBr, cm^{-1}) ν_{max} : 3445 (asym, NH_2), 3362 (sym, NH_2), 2247 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.86 (s, 1H, $\text{N}_{11}\text{-H}$), 7.57-7.54 (m, 2H, C_4' & $\text{C}_5'\text{-H}$), 7.38-7.26 (m, 3H, C_7 , C_9 & $\text{C}_{10}\text{-H}$), 5.19 (s, 2H, NH_2), 2.89-2.79 (m, 4H, $\text{C}_5\text{-2H}$ & $\text{C}_6\text{-2H}$), 2.58 (s, 3H, $\text{C}_8\text{-CH}_3$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 154.1 (C_2), 147.3 ($\text{C}_{11\text{b}}$), 145.2 (C_4), 144.8 (C_1'), 136.1 ($\text{C}_{10\text{a}}$), 135.4 (C_4'), 134.9 (C_5'), 132.0 ($\text{C}_{4\text{a}}$), 130.4 (C_8), 128.8 ($\text{C}_{6\text{b}}$), 124.6 ($\text{C}_{11\text{a}}$), 122.5 (C_9), 120.3 (C_7), 117.5 ($\text{C}_{6\text{a}}$), 115.7 ($\text{C}\equiv\text{N}$), 114.9 ($\text{C}\equiv\text{N}$), 113.7 (C_5'), , 111.7 (C_{10}), 95.9 (C_3), 94.7 (C_1), 29.2 (C_5), 25.1 (C_6), 22.0 ($\text{C}_8\text{-CH}_3$); MS: m/z (%) 458 (M^+ 100), 460 ($\text{M}+2$); Anal.Calcd.for $\text{C}_{23}\text{H}_{15}\text{BrN}_4\text{S}$: C, 60.14; H, 3.29; N, 12.20. Found: C, 60.12; H, 3.31; N, 12.19 %

2-Amino-8-chloro-4-phenyl-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (4b)

Yellow solid; yield: 80%; m.p. 231-233 °C; IR (KBr, cm^{-1}) ν_{max} : 3441 (asym, NH_2), 3329 (sym, NH_2), 2241 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.79 (s, 1H, $\text{N}_{11}\text{-H}$), 7.49-7.38 (m, 3H, C_7 , C_9 & $\text{C}_{10}\text{-H}$), 7.34-7.29 (m, 5H, C_2' , C_3' , C_4' , C_5' & $\text{C}_6'\text{-H}$), 5.27 (s, 2H, NH_2), 2.85-2.79 (m, 4H, $\text{C}_5\text{-2H}$ & $\text{C}_6\text{-2H}$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 158.2 (C_2), 146.7 ($\text{C}_{11\text{b}}$), 144.3 (C_4), 137.3 ($\text{C}_{10\text{a}}$), 131.4 (C_1'), 130.3 (C_3' & C_5'), 128.6 ($\text{C}_{4\text{a}}$), 127.7 (C_8), 127.0 (C_2' & C_6'), 126.8 (C_4'), 126.0 ($\text{C}_{6\text{b}}$), 123.4 ($\text{C}_{11\text{a}}$), 121.1 (C_9), 120.3 (C_7), 117.2 ($\text{C}_{6\text{a}}$), 115.7 ($\text{C}\equiv\text{N}$), 114.6 ($\text{C}\equiv\text{N}$), 111.5 (C_{10}), 96.1 (C_3), 94.2 (C_1), 30.2 (C_5), 25.2 (C_6); MS: m/z (%) 394 (M^+ 100); Anal.Calcd.for $\text{C}_{24}\text{H}_{15}\text{ClN}_4$: C, 73.00; H, 3.83; N, 14.19. Found : C, 73.02; H, 3.85; N, 14.23 %

2-Amino-8-chloro-4-(4'-bromo-phenyl)-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (5b)

Yellow solid; yield: 80%; m.p. 243-245 °C; IR (KBr, cm^{-1}) ν_{max} : 3451 (asym, NH_2), 3361 (sym, NH_2), 2216 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.64 (s, 1H, $\text{N}_{11}\text{-H}$), 7.45-7.37 (m, 3H, C_7 , C_9 & $\text{C}_{10}\text{-H}$), 7.32-7.25 (m, 4H, C_2' , C_3' , C_5' & $\text{C}_6'\text{-H}$), 5.31 (s, 2H, NH_2), 2.74-2.69 (m, 4H, $\text{C}_5\text{-2H}$ & $\text{C}_6\text{-2H}$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 153.2 (C_2), 147.1 ($\text{C}_{11\text{b}}$), 146.5 (C_4), 138.3 ($\text{C}_{10\text{a}}$), 132.4 (C_1'), 131.0 (C_2' & C_6'), 130.0 ($\text{C}_{4\text{a}}$), 129.1 (C_8), 127.2 ($\text{C}_{6\text{b}}$), 126.4 (C_4'), 125.9 (C_3' & C_5'), 124.3 ($\text{C}_{11\text{a}}$), 122.1 (C_9), 119.4 (C_7), 116.4 ($\text{C}_{6\text{a}}$), 115.3 ($\text{C}\equiv\text{N}$), 114.7 ($\text{C}\equiv\text{N}$), 110.7 (C_{10}), 95.2 (C_3), 94.0 (C_1), 28.2 (C_5), 24.0 (C_6); MS: m/z (%) 473 (M^+ 100%), 475 ($\text{M}+2$); Anal.Calcd.for $\text{C}_{24}\text{H}_{14}\text{BrClN}_4$: C, 60.85; H, 2.98; N, 11.83. Found : C, 60.82; H, 2.96; N, 11.87 %

2-Amino-8-chloro-4-(4'-dimethylamino-phenyl)-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (6b)

Yellow solid; yield: 80%; m.p. 236-238 °C; IR (KBr, cm^{-1}) ν_{max} : 3439 (asym, NH_2), 3357 (sym, NH_2), 2228 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.83 (s, 1H, $\text{N}_{11}\text{-H}$), 7.51-7.47 (m, 3H, C_7 , C_9 & $\text{C}_{10}\text{-H}$), 7.44-7.39 (m, 4H, C_2' , C_3' , C_5' & $\text{C}_6'\text{-H}$), 5.46 (s, 2H, NH_2), 3.22 (s, 6H, $\text{N}(\text{CH}_3)_2$), 2.87-2.80 (m, 4H, $\text{C}_5\text{-2H}$ & $\text{C}_6\text{-2H}$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 154.2 (C_4'), 152.2 (C_2), 147.4 ($\text{C}_{11\text{b}}$), 146.1 (C_4), 137.3 ($\text{C}_{10\text{a}}$), 131.0 (C_2' & C_6'), 129.8 ($\text{C}_{4\text{a}}$), 129.0 (C_8), 127.6 ($\text{C}_{6\text{b}}$), 122.9 (C_1'), 122.7 (C_9), 121.9 ($\text{C}_{11\text{a}}$), 119.0 (C_7), 116.9 ($\text{C}_{6\text{a}}$), 115.2 ($\text{C}\equiv\text{N}$), 114.0 ($\text{C}\equiv\text{N}$), 113.9 (C_3' & C_5'), 111.3 (C_{10}), 95.6 (C_3), 94.0 (C_1), 43.5 ($\text{N}(\text{CH}_3)_2$), 30.1 (C_5), 25.3 (C_6); MS: m/z (%) 437 (M^+ 100); Anal.Calcd.for $\text{C}_{26}\text{H}_{20}\text{ClN}_5$: C, 71.31; H, 4.60; N, 15.99. Found : C, 71.33; H, 4.63; N, 16.00 %

2-Amino-8-chloro-4-(pyridin-3'-yl)-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (7b)

Yellow solid; yield: 81%; m.p. 230-232 °C IR (KBr, cm^{-1}) ν_{max} : 3456 (asym, NH_2), 3329 (sym, NH_2), 2229 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.64 (s, 1H, $\text{N}_{11}\text{-H}$), 7.79-7.76 (m, 4H, C_2' , C_4' , C_5' & $\text{C}_6'\text{-H}$), 7.45-7.39 (m, 3H, C_7 , C_9 & $\text{C}_{10}\text{-H}$), 5.39 (s, 2H, NH_2), 3.01- 2.97(m, 4H, $\text{C}_5\text{-2H}$ & $\text{C}_6\text{-2H}$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 154.1 (C_2), 150.8 (C_2'), 148.9 (C_4'), 148.5 ($\text{C}_{11\text{b}}$), 146.1 (C_4), 139.5 (C_6'), 137.8 ($\text{C}_{10\text{a}}$), 136.6 (C_1'), 131.3 ($\text{C}_{4\text{a}}$), 130.2 (C_8), 129.0 ($\text{C}_{6\text{b}}$), 127.1 (C_5'), 123.8 ($\text{C}_{11\text{a}}$), 123.2 (C_9), 120.0 (C_7), 118.2 ($\text{C}_{6\text{a}}$), 115.1 ($\text{C}\equiv\text{N}$), 114.8 ($\text{C}\equiv\text{N}$), 110.7 (C_{10}), 95.9 (C_3), 94.6 (C_1), 28.6 (C_5), 25.1 (C_6); MS: m/z (%) 395 (M^+ 100); Anal.Calcd.for $\text{C}_{23}\text{H}_{14}\text{ClN}_5$: C, 69.79; H, 3.56; N, 17.69. Found : C, 69.76; H, 3.58; N, 17.66 %

2-Amino-4-(5'-bromothiophen-2'-yl)-8-chloro-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (8b)

Yellow solid; yield: 82%; m.p. 242-244 °C; IR (KBr, cm^{-1}) ν_{max} : 3456 (asym, NH_2), 3329 (sym, NH_2), 2229 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.71 (s, 1H, $\text{N}_{11}\text{-H}$), 7.64-7.56 (m, 2H, C_4' & $\text{C}_5'\text{-H}$), 7.45-7.36 (m, 3H, C_7 , C_9 & $\text{C}_{10}\text{-H}$), 5.44 (s, 2H, NH_2), 2.89-2.84 (m, 4H, $\text{C}_5\text{-2H}$ & $\text{C}_6\text{-2H}$); ^{13}C NMR (125 MHz, CDCl_3) (ppm) δ_{C} : 153.5 (C_2), 147.8 ($\text{C}_{11\text{b}}$), 146.6 (C_4), 145.1 (C_1'), 137.3 ($\text{C}_{10\text{a}}$), 136.7 (C_4'), 135.2 (C_5'), 132.6 ($\text{C}_{4\text{a}}$), 131.6 (C_8), 129.0 ($\text{C}_{6\text{b}}$), 124.8 ($\text{C}_{11\text{a}}$), 122.7 (C_9), 121.1 (C_7), 117.9 ($\text{C}_{6\text{a}}$), 115.8 ($\text{C}\equiv\text{N}$), 114.8 (C_5'), 114.4 ($\text{C}\equiv\text{N}$), 111.2 (C_{10}), 96.1 (C_3), 95.1 (C_1), 29.6 (C_5), 25.5 (C_6); MS: m/z (%) 400 (M^+ 100%), 402 ($\text{M}+2$); Anal.Calcd.for $\text{C}_{22}\text{H}_{12}\text{BrN}_4\text{S}$: C, 55.07; H, 2.52; N, 11.68. Found: C, 55.05; H, 2.49; N, 11.71 %

2-Amino-4-phenyl-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (4c)

Yellow solid; yield: 81%; m.p. 228-230 °C; IR (KBr, cm^{-1}) ν_{max} : 3443 (asym, NH_2), 3361 (sym, NH_2), 2218 ($\text{C}\equiv\text{N}$); ^1H NMR (500 MHz, CDCl_3) (ppm) δ_{H} : 8.79 (s, 1H, $\text{N}_{11}\text{-H}$), 7.64-7.52 (m, 4H, C_7 , C_8 , C_9 & $\text{C}_{10}\text{-H}$), 7.47-7.32 (m, 5H, C_2' , C_3' , C_4' , C_5' & $\text{C}_6'\text{-H}$), 5.22 (s, 2H, NH_2), 2.95-

2.82 (m, 4H, C₅-2H & C₆-2H); ¹³C NMR (125 MHz, CDCl₃) (ppm) δ_C: 157.9 (C₂), 145.3 (C_{11b}), 144.7 (C₄), 138.2 (C_{10a}), 131.8 (C_{1'}), 131.1 (C_{3'} & C_{5'}), 129.3 (C_{4a}), 128.6 (C₈), 126.9 (C_{2'} & C_{6'}), 126.5 (C_{4'}), 125.7 (C_{6b}), 124.1 (C_{11a}), 122.4 (C₉), 121.1 (C₇), 118.1 (C_{6a}), 115.4 (C≡N), 114.7 (C≡N), 110.1 (C₁₀), 96.8 (C₃), 95.0 (C₁), 29.7 (C₅), 24.9 (C₆); MS: m/z (%) 360 (M⁺ 100); Anal.Calcd.for C₂₄H₁₆N₄: C, 79.98; H, 4.47; N, 15.55. Found: C, 79.96; H, 4.49; N, 15.59 %

2-Amino-4-(4'-bromo-phenyl)-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (5c)

Yellow solid; yield: 80%; m.p. 237-239 °C; IR (KBr, cm⁻¹)_v_{max}: 3459 (asym, NH₂), 3342 (sym, NH₂), 2227 (C≡N); ¹H NMR (500 MHz, CDCl₃) (ppm) δ_H: 8.71 (s, 1H, N₁₁-H), 7.54-7.47 (m, 4H, C₇, C₈, C₉ & C₁₀ -H), 7.42-7.38 (m, 4H, C_{2'}, C_{3'}, C_{5'} & C_{6'}-H), 5.37 (s, 2H, NH₂), 2.80-2.76 (m, 4H, C₅-2H & C₆-2H); ¹³C NMR (125 MHz, CDCl₃) (ppm) δ_C: 155.1 (C₂), 148.6 (C_{11b}), 147.2 (C₄), 138.3 (C_{10a}), 132.3 (C_{1'}), 131.8 (C_{2'} & C_{6'}), 130.9 (C_{4a}), 130.0 (C₈), 128.6 (C_{6b}), 127.5 (C_{4'}), 126.2 (C_{3'} & C_{5'}), 125.2 (C_{11a}), 123.5 (C₉), 120.2 (C₇), 117.1 (C_{6a}), 115.7 (C≡N), 114.7 (C≡N), 110.4 (C₁₀), 95.9 (C₃), 94.7 (C₁), 29.6 (C₅), 25.1 (C₆); MS: m/z (%) 439 (M⁺ 100%), 441 (M+2); Anal.Calcd.for C₂₄H₁₅BrN₄: C, 65.62; H, 3.44; N, 12.75. Found : C, 65.60; H, 3.43; N, 12.78 %

2-Amino-4-(4'-dimethylamino-phenyl)-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (6c)

Yellow solid; yield: 81%; m.p. 236-238 °C; IR (KBr, cm⁻¹)_v_{max}: 3432 (asym, NH₂), 3363 (sym, NH₂), 2230 (C≡N); ¹H NMR (500 MHz, CDCl₃) (ppm) δ_H: 8.69 (s, 1H, N₁₁-H), 7.50-7.45 (m, 4H, C₇, C₈, C₉ & C₁₀ -H), 7.37-7.32 (m, 4H, C_{2'}, C_{3'}, C_{5'} & C_{6'}-H), 5.41 (s, 2H, NH₂), 3.20 (s, 6H, N(CH₃)₂), 2.82-2.74 (m, 4H, C₅-2H & C₆-2H); ¹³C NMR (125 MHz, CDCl₃) (ppm) δ_C: 156.1 (C_{4'}), 151.9 (C₂), 146.2 (C_{11b}), 145.1 (C₄), 138.6 (C_{10a}), 132.2 (C_{2'} & C_{6'}), 130.5 (C_{4a}), 129.3 (C₈), 128.3 (C_{6b}), 124.1 (C_{1'}), 122.9 (C_{11a}), 121.3 (C₉), 120.3 (C₇), 117.93 (C_{6a}), 115.6 (C≡N), 114.9 (C≡N), 113.3 (C_{3'} & C_{5'}), 110.7 (C₁₀), 96.0 (C₃), 95.5 (C₁), 42.7 (N(CH₃)₂), 29.8 (C₅),

26.1 (C₆); MS: m/z (%) 403 (M⁺ 100); Anal.Calcd.for C₂₆H₂₁N₅: C, 77.40; H, 5.25; N, 17.36.
Found : C, 77.38; H, 5.22; N, 17.35 %

2-Amino-4-(pyridin-3'-yl)-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (7c)

Yellow solid; yield: 82%; m.p. 235-237 °C; IR (KBr, cm⁻¹)_v_{max}: 3462 (asym, NH₂), 3359 (sym, NH₂), 2216 (C≡N); ¹H NMR (500 MHz, CDCl₃) (ppm) δ_H: 8.67 (s, 1H, N₁₁-H), 7.82-7.75 (m, 4H, C_{2'}, C_{4'}, C_{5'} & C_{6'}-H), 7.47-7.38 (m, 4H, C₇, C₈, C₉ & C₁₀-H), 5.41 (s, 2H, NH₂), 2.87-2.79 (m, 4H, C₅-2H & C₆-2H); ¹³C NMR (125 MHz, CDCl₃) (ppm) δ_C: 155.1 (C₂), 151.1 (C_{2'}), 149.3 (C_{4'}), 147.4 (C_{11b}), 146.9 (C₄), 140.3 (C_{6'}), 138.2 (C_{10a}), 137.1 (C_{1'}), 131.8 (C_{4a}), 131.6 (C₈), 130.1 (C_{6b}), 127.8 (C_{5'}), 124.1 (C_{11a}), 123.8 (C₉), 121.1 (C₇), 117.8 (C_{6a}), 115.6 (C≡N), 114.5 (C≡N), 109.2 (C₁₀), 96.6 (C₃), 94.7 (C₁), 29.2 (C₅), 25.8 (C₆); MS: m/z (%) 361 (M⁺ 100); Anal.Calcd.for C₂₃H₁₅N₅: C, 76.44; H, 4.16; N, 19.38. Found : C, 76.40; H, 4.12; N, 19.36 %

2-Amino-4(5'-bromothiophen-2'-yl)-5,6-dihydro-11H-benzo[a]carbazole-1,3-dicarbonitrile (8c)

Yellow solid; yield: 80%; m.p. 239-241 °C; IR (KBr, cm⁻¹)_v_{max}: 3457 (asym, NH₂), 3343 (sym, NH₂), 2228 (C≡N); ¹H NMR (500 MHz, CDCl₃) (ppm) δ_H: 8.71 (s, 1H, N₁₁-H), 7.76-7.64 (m, 2H, C_{4'} & C_{5'}-H), 7.45-7.36 (m, 4H, C₇, C₈, C₉ & C₁₀-H), 5.40 (s, 2H, NH₂), 2.92-2.89 (m, 4H, C₅-2H & C₆-2H); ¹³C NMR (125 MHz, CDCl₃) (ppm) δ_C: 154.2 (C₂), 148.3 (C_{11b}), 147.2 (C₄), 145.9 (C_{1'}), 136.1 (C_{10a}), 135.9 (C_{4'}), 135.7 (C_{5'}), 133.1 (C_{4a}), 132.5 (C₈), 130.0 (C_{6b}), 125.1 (C_{11a}), 123.0 (C₉), 121.9 (C₇), 118.0 (C_{6a}), 115.4 (C≡N), 114.9 (C_{5'}), 114.3 (C≡N), 111.9 (C₁₀), 96.8 (C₃), 95.6 (C₁), 29.8 (C₅), 25.9 (C₆); MS: m/z (%) 445 (M⁺ 100), 447 (M+2); Anal.Calcd.for C₂₂H₁₃BrN₄S: C, 59.33; H, 2.94; N, 12.58. Found : C, 59.30; H, 2.93; N, 12.54 %

DETAILS OF THE CRYSTAL STRUCTURE COMPOUND **8b**

Table III Crystal data and structure refinement data.

	8b
CCDC deposit number	897288
Empirical formula	$\text{C}_{22}\text{H}_{12}\text{BrClN}_4\text{S}\cdot\text{C}_2\text{H}_6\text{O}$
Formula weight	525.84
Temperature	90
Wavelength	$\lambda = 0.71073 \text{ \AA}$
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell Dimensions	
a(Å)	10.4991 (15)
b(Å)	26.977 (3) Å
c(Å)	7.8845 (10) Å
$\alpha(^{\circ})$	90
$\beta(^{\circ})$	91.944 (5) $^{\circ}$
$\gamma(^{\circ})$	90
Volume(Å ³)	2231.9 (5)
Z	4
Density (calculated) Mg/m ³	1.565
Absorption coefficient(mm ⁻¹)	2.080
F(000)	1064
Theta range for data collection	2.7 to 40.0 $^{\circ}$

	-17<=h<=17,
Index ranges	-45<=k<=45,
	-6<=l<=14
Reflections collected / unique	31583/ 11238
Completeness to theta (max)	0.799
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11238/ 1 / 302
Goodness-of-fit on F ²	1.032
Final R indices [I>2σ(I)]	R ₁ = 0.0325, wR ₂ = 0.0802
R indices (all data)	R ₁ = 0.0461, wR ₂ = 0.0862
Largest diff. peak and hole	1.19 and -0.61 e. Å ⁻³

data_8b

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treatment of cell esds is used for estimating esds involving l.s. planes.

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 C10 C9 H9B 109.2 . . ?
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IR SPECTRUM OF COMPOUND 4a

¹H NMR SPECTRUM OF COMPOUND 4a

^1H NMR SPECTRUM OF COMPOUND 5a

^1H NMR SPECTRUM OF COMPOUND 6a

^1H NMR SPECTRUM OF COMPOUND 7a

^1H NMR SPECTRUM OF COMPOUND 8a

^1H NMR SPECTRUM OF COMPOUND 4b

^1H NMR SPECTRUM OF COMPOUND 5b

¹H NMR SPECTRUM OF COMPOUND 6b

¹H NMR SPECTRUM OF COMPOUND 7b

^1H NMR SPECTRUM OF COMPOUND 8b

^1H NMR SPECTRUM OF COMPOUND 4c

^1H NMR SPECTRUM OF COMPOUND 5c

^1H NMR SPECTRUM OF COMPOUND 6c

^1H NMR SPECTRUM OF COMPOUND 7c

^1H NMR SPECTRUM OF COMPOUND 8c

^{13}C NMR SPECTRUM OF COMPOUND 4a

^{13}C NMR SPECTRUM OF COMPOUND 5a

^{13}C NMR SPECTRUM OF COMPOUND 6a

^{13}C NMR SPECTRUM OF COMPOUND 7a

^{13}C NMR SPECTRUM OF COMPOUND 8a

^{13}C NMR SPECTRUM OF COMPOUND 4b

^{13}C NMR SPECTRUM OF COMPOUND 5b

^{13}C NMR SPECTRUM OF COMPOUND 6b

^{13}C NMR SPECTRUM OF COMPOUND 7b

^{13}C NMR SPECTRUM OF COMPOUND 8b

^{13}C NMR SPECTRUM OF COMPOUND 4c

^{13}C NMR SPECTRUM OF COMPOUND 5c

^{13}C NMR SPECTRUM OF COMPOUND 6c

^{13}C NMR SPECTRUM OF COMPOUND 7c

^{13}C NMR SPECTRUM OF COMPOUND 8c