Supplementary Content

Novel 4-aryl-2-amino-6-(naphthalene-1-yl)-3-cyanopyridine derivatives as potential organic fluorescent materials prepared under microwave irradiation via “three-component” Domino reactions

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Experimental:

Compound characterization

4a: 2-amino-6-(naphthalen-1-yl)-4-phenyl-3-cyanopyridine

The compound was obtained as yellow crystals, mp 165-167 °C; IR (KBr, ν , cm⁻¹): 3390, 3306 ν (NH₂, Ar), 3171, 3057 ν (=C-H), 2212 ν (CN), 1634, 1617, 1492 ν (C=C, Ar), 1449 ν (C=N), 773, 696 δ (C-H) cm⁻¹; ¹H NMR (300 MHz, CDCl₃) (δ , ppm): 5.64 (s, 2H, NH₂), 7.07(s, 1H, ArH), 7.48-7.49(m, 1H, ArH), 7.49-7.55(m, 5H, ArH), 7.62-7.68(m, 3H, ArH), 7.93-7.98(m, 2H, ArH), 8.14-8.18(m, 1H, ArH); ¹³C NMR (100 MHz, CDCl₃) (δ , ppm): 88.3, 115.6, 117.0, 125.2, 125.4, 126.2, 126.8, 127.3, 128.3, 128.6, 129.0, 129.8, 130.0, 130.8, 134.0, 136.6, 137.2, 154.9, 160.3, 162.0; HRMS(ESI) m/z: calc. for: C₂₂H₁₅N₃, 322.1339 [M+H]⁺; found: 322.1331; Anal.calcd. for C₂₂H₁₅N₃: C 82.22, H 4.70, N 13.08; found C 82.58, H 4.54, N 12.81.

4b: 2-amino-6-(naphthalen-1-yl)-4-(3-methylphenyl)-3-cyanopyridine

The compound was obtained as yellow crystals, mp 171-173 °C; IR (KBr, ν , cm^{-1}): 3398, 3307 $\nu(\text{NH}_2, \text{Ar})$, 3176 $\nu(\text{=C-H})$, 2212 $\nu(\text{CN})$, 1635, 1615, 1491 $\nu(\text{C=C, Ar})$, 1442 $\nu(\text{C=N})$, 869, 780, 704 $\delta(\text{C-H}) \text{ cm}^{-1}$; ^1H NMR (300 MHz, CDCl_3) (δ , ppm): 2.44 (s, 3H, CH_3), 5.44 (s, 2H, NH_2), 7.07 (s, 1H, ArH), 7.32 (d, $J=8$ Hz, 1H, ArH), 7.38-7.43 (m, 1H, ArH), 7.46-7.51 (m, 2H, ArH), 7.52-7.58 (m, 3H, ArH), 7.62-7.65 (m, 1H, ArH), 7.90-7.96 (m, 2H, ArH), 8.13-8.17 (t, $J=7$ Hz, 1H, ArH); ^{13}C NMR (100 MHz, CDCl_3) (δ , ppm): 21.5, 88.3, 115.7, 117.0, 125.2, 125.3, 125.4, 126.2, 126.8, 127.3, 128.5, 128.9, 129.8, 130.7, 134.0, 136.7, 137.4, 138.8, 155.0, 160.2, 162.0; HRMS(ESI) m/z : calc. for: $\text{C}_{23}\text{H}_{17}\text{N}_3$, 336.1495 $[\text{M}+\text{H}]^+$; found: 336.1477; Anal. calcd. for $\text{C}_{23}\text{H}_{17}\text{N}_3$: C 82.36, H 5.11, N 12.53; found C 82.32, H 5.20, N 12.27.

4c: 2-amino-4-(2-fluorophenyl)-6-(naphthalen-1-yl)-3-cyanopyridine

The compound was obtained as yellow crystals, mp 165-167 °C; IR (KBr, ν , cm^{-1}): 3472, 3297 $\nu(\text{NH}_2, \text{Ar})$, 3169 $\nu(\text{=C-H})$, 2206 $\nu(\text{CN})$, 1616, 1549, 1493 $\nu(\text{C=C, Ar})$, 1451 $\nu(\text{C=N})$, 803, 764 $\delta(\text{C-H}) \text{ cm}^{-1}$; ^1H NMR (300 MHz, CDCl_3) (δ , ppm): 5.49 (s, 2H, NH_2), 7.06 (s, 1H, ArH), 7.24-7.26 (m, 1H, ArH), 7.29-7.32 (m, 1H, ArH), 7.49-7.57 (m, 5H, ArH), 7.63-7.66 (m, 1H, ArH), 7.89-7.96 (m, 2H, ArH), 8.16-8.19 (m, 1H, ArH); ^{13}C NMR (100 MHz, CDCl_3) (δ , ppm): 89.6, 116.4, 116.8, 124.6, 125.2, 125.3, 126.2, 126.8, 127.5, 128.6, 129.9, 130.6, 130.6, 130.7, 131.8, 134.0, 137.0, 149.3, 159.8, 162.1; HRMS(ESI) m/z : calc. for: $\text{C}_{22}\text{H}_{14}\text{FN}_3$, 340.1245 $[\text{M}+\text{H}]^+$; found: 340.1243; Anal. calcd. for $\text{C}_{22}\text{H}_{14}\text{FN}_3$: C 77.86, H 4.16, N 12.38; found C 77.62, H 4.34, N 12.54.

4d: 2-amino-4-(2,4-dichlorophenyl)-6-(naphthalen-1-yl)-3-cyanopyridine

The compound was obtained as yellow crystals, mp 139-141 °C; IR (KBr, ν , cm^{-1}): 3470, 3350 $\nu(\text{NH}_2, \text{Ar})$, 3170 $\nu(\text{=C-H})$, 3060 $\nu(\text{=C-H})$, 2212 $\nu(\text{CN})$, 1624, 1590, 1570, 1544, 1480 $\nu(\text{C=C, Ar})$, 1440 $\nu(\text{C=N})$, 802, 778 $\delta(\text{C-H}) \text{ cm}^{-1}$; ^1H NMR (300 MHz, CDCl_3) (δ , ppm): 5.50 (s, 2H, NH_2), 7.00 (s, 1H, ArH), 7.35-7.42 (m, 2H, ArH), 7.52-7.57 (m, 5H, ArH), 7.64-7.66 (m, 1H, ArH), 7.90-7.96 (m, 2H, ArH), 8.15-8.19 (m, 1H, ArH); ^{13}C NMR (100 MHz, CDCl_3) (δ , ppm): 89.9, 116.0, 116.6, 125.2, 125.3, 126.2, 126.9, 127.5, 127.6, 128.6, 130.1, 130.3, 131.2, 133.3, 134.0, 136.3, 136.9, 151.5, 159.7, 162.1; HRMS(ESI) m/z : calc. for: $\text{C}_{22}\text{H}_{13}\text{Cl}_2\text{N}_3$, 390.0559 $[\text{M}+\text{H}]^+$; found: 390.0572; Anal. calcd. for $\text{C}_{22}\text{H}_{13}\text{Cl}_2\text{N}_3$: C 67.71, H 3.36, N 10.77; found C 67.52, H 3.48, N 10.91.

4e: 2-amino-4-(furan-2-yl)-6-(naphthalen-1-yl)-3-cyanopyridine

The compound was obtained as yellow crystals, mp 171-173 °C; IR (KBr, ν , cm^{-1}): 3471, 3351 $\nu(\text{NH}_2, \text{Ar})$, 3143 $\nu(\text{=C-H})$, 2209 $\nu(\text{CN})$, 1623, 1556, 1506, 1484 $\nu(\text{C=C, Ar})$, 1452 $\nu(\text{C=N})$, 807, 793, 777, 746

$\delta(\text{C-H}) \text{ cm}^{-1}$; ^1H NMR (300 MHz, CDCl_3) (δ , ppm): 5.46 (s, 2H, NH_2), 6.61-6.62 (m, 1H, ArH), 7.39 (s, 1H, ArH), 7.50-7.62 (m, 6H, ArH), 7.92-7.96 (m, $J=6$ Hz, 2H, ArH), 8.10-8.13 (t, 1H, ArH); ^{13}C NMR (100 MHz, CDCl_3) (δ , ppm): 83.0, 110.9, 112.7, 113.5, 117.4, 125.2, 125.4, 126.2, 126.8, 127.2, 128.5, 129.8, 130.7, 134.0, 137.5, 141.4, 144.7, 148.8, 160.3, 162.3; HRMS(ESI) m/z : calc. for: $\text{C}_{20}\text{H}_{13}\text{N}_3\text{O}$, 312.1131 $[\text{M}+\text{H}]^+$; found: 312.1123; Anal.calcd. for $\text{C}_{20}\text{H}_{13}\text{N}_3\text{O}$: C 77.16, H 4.21, N 13.50; found C 77.42, H 4.35, N 13.37.

4f: 2-amino-4-(3-fluorophenyl)-6-(naphthalen-1-yl)-3-cyanopyridine

The compound was obtained as yellow crystals, mp 162-164 °C; IR (KBr, ν , cm^{-1}): 3459, 3292 $\nu(\text{NH}_2, \text{Ar})$, 3157 $\nu(\text{=C-H})$, 2212 $\nu(\text{CN})$, 1628, 1549, 1488 $\nu(\text{C=C, Ar})$, 1446 $\nu(\text{C=N})$, 791, 780, 709 $\delta(\text{C-H}) \text{ cm}^{-1}$; ^1H NMR (300 MHz, CDCl_3) (δ , ppm): 5.51 (s, 2H, NH_2), 7.04 (s, 1H, ArH), 7.17-7.18 (m, 1H, ArH), 7.20- 7.37 (m, 1H, ArH), 7.44-7.57 (m, ArH, 5H), 7.62-7.65 (m, 1H, ArH), 7.91-7.94 (m, 2H, ArH), 8.13-8.16 (m, 1H, ArH); ^{13}C NMR (100 MHz, CDCl_3) (δ , ppm): 88.1, 115.5, 116.8, 124.1, 125.2, 125.3, 126.2, 126.9, 127.4, 128.4, 128.6, 130.0, 130.7, 131.0, 134.0, 137.0, 138.7, 153.4, 160.2, 162.4; HRMS(ESI) m/z : calc. for: $\text{C}_{22}\text{H}_{14}\text{FN}_3$, 340.1245 $[\text{M}+\text{H}]^+$; found: 340.1241; Anal.calcd. for $\text{C}_{22}\text{H}_{14}\text{FN}_3$: C 77.86, H 4.16, N 12.38; found C 77.56, H 4.24, N 12.49.

Spectra of all compounds:

Fig S1 The IR spectrum of the compound **4a**

Fig S2 The IR spectrum of the compound **4b**

Fig S3 The IR spectrum of the compound **4c**

Fig S4 The IR spectrum of the compound **4d**

Fig S5 The IR spectrum of the compound **4e**

Fig S6 The IR spectrum of the compound **4f**

Fig S7 The ^1H -NMR of the compound **4a**

Fig S9 The ^1H -NMR of the compound **4c**

Fig S10 The ^1H -NMR of the compound **4d**

Fig S11 The ^1H -NMR of the compound **4e**

Fig S12 The ^1H -NMR of the compound **4f**

Fig S13 The ^{13}C -NMR of the compound **4a**

Fig S14 The ^{13}C -NMR of the compound **4b**

Fig S15 The ^{13}C -NMR of the compound **4c**

Fig S16 The ^{13}C -NMR of the compound **4d**

Fig S17 The ^{13}C -NMR of the compound **4e**

Fig S18 The ^{13}C -NMR of the compound **4f**

Fig S19 The HRMS (ESI) of the compound **4a**

Fig S20 The HRMS (ESI) of the compound **4b**

Fig S21 The HRMS (ESI) of the compound **4c**

Fig S22 The HRMS (ESI) of the compound **4d**

Fig S23 The HRMS (ESI) of the compound **4e**

Fig S24 The HRMS (ESI) of the compound **4f**