

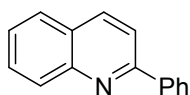
Supporting information for

Palladium-Catalyzed Synthesis of Quinolines from Allyl
alcohols and Anilines

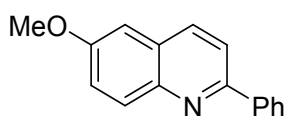
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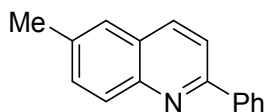
Characterization data for products



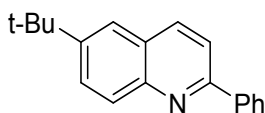
2-phenylquinoline (3aa)¹ White solid. Mp 85-86 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.26 – 8.07 (m, 4H), 7.84 (dd, *J* = 20.0, 8.3 Hz, 2H), 7.72 (t, *J* = 7.7 Hz, 1H), 7.52 (dd, *J* = 7.5, 4.9 Hz, 3H), 7.46 (t, *J* = 7.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 157.4, 148.3, 139.7, 136.8, 129.7, 129.4, 128.9, 127.6, 127.5, 127.2, 126.3, 119.0.



6-methoxy-2-phenylquinoline (3ba)¹ White solid. Mp 134-135 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.30 – 8.04 (m, 4H), 7.85 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.44 (dd, *J* = 24.9, 8.4 Hz, 2H), 7.11 (s, 1H), 3.97 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 157.7, 155.0, 144.3, 139.7, 135.5, 131.1, 128.9, 128.8, 128.1, 127.3, 122.3, 119.2, 105.0, 55.5.

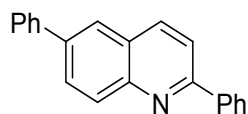


6-methyl-2-phenylquinoline (3ca)¹ White solid. Mp 89-90 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.16 – 8.09 (m, 2H), 8.05 (d, *J* = 8.5 Hz, 1H), 7.99 – 7.94 (m, 1H), 7.71 (d, *J* = 8.6 Hz, 1H), 7.54 – 7.43 (m, 4H), 7.43 – 7.33 (m, 1H), 2.45 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 156.5, 146.9, 139.9, 136.1, 136.1, 132.0, 129.5, 129.2, 128.9, 127.5, 127.3, 126.4, 118.9, 21.6.

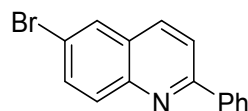


6-(tert-butyl)-2-phenylquinoline (3da)¹ White solid. Mp 109-110 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.24 – 8.11 (m, 4H), 7.84 (td, *J* = 6.7, 3.2 Hz, 2H), 7.75 (s, 1H), 7.52 (td, *J* = 6.6, 3.4 Hz, 2H), 7.46 (dd,

$J = 8.4, 6.4$ Hz, 1H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, CDCl_3) δ 156.7, 149.3, 137.1, 129.3, 129.0, 128.9, 127.6, 126.9, 122.5, 119.0, 35.0, 31.2.

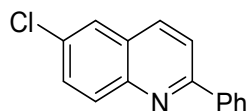


2,6-diphenylquinoline (3ea)¹ White solid. Mp 203-204 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.30 – 8.15 (m, 4H), 8.06 – 7.97 (m, 2H), 7.90 (dd, $J = 8.8, 2.3$ Hz, 1H), 7.74 (d, $J = 7.6$ Hz, 2H), 7.59 – 7.45 (m, 5H), 7.44 – 7.35 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.3, 147.7, 140.4, 139.6, 139.1, 137.0, 130.1, 129.4, 129.4, 129.0, 128.9, 127.7, 127.6, 127.4, 127.4, 125.2, 119.4.

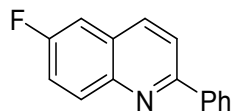


6-bromo-2-phenylquinoline (3fa)¹ Light yellow solid. Mp 129-130 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.14 (t, $J = 9.0$ Hz, 3H), 8.05 (d, $J = 9.0$ Hz, 1H), 7.99 (s, 1H), 7.89 (d, $J = 8.6$ Hz, 1H), 7.79 (d, $J = 9.0$ Hz, 1H), 7.60 – 7.41 (m, 3H).

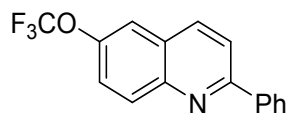
^{13}C NMR (101 MHz, CDCl_3) δ 157.6, 146.7, 139.1, 135.8, 133.1, 131.4, 129.6, 129.5, 128.9, 128.2, 127.5, 120.1, 119.8.



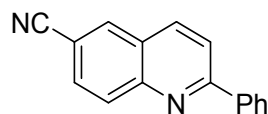
6-chloro-2-phenylquinoline (3ga)¹ White solid. Mp 109-110 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.10 – 8.04 (m, 2H), 8.01 (dt, $J = 9.0, 0.6$ Hz, 1H), 7.88 (dd, $J = 8.7, 0.8$ Hz, 1H), 7.69 (d, $J = 8.6$ Hz, 1H), 7.62 (d, $J = 2.4$ Hz, 1H), 7.55 (dd, $J = 9.0, 2.4$ Hz, 1H), 7.49 – 7.37 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.4, 146.6, 139.2, 135.7, 131.9, 131.3, 130.5, 129.6, 128.9, 127.7, 127.5, 126.2, 119.6.



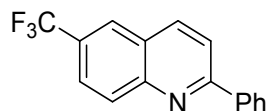
6-fluoro-2-phenylquinoline (3ha)¹ White solid. Mp 100-101 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.26 – 8.06 (m, 4H), 7.88 (d, $J = 8.5$ Hz, 1H), 7.63 – 7.34 (m, 5H). ^{13}C NMR (101 MHz, CDCl_3) δ 161.6, 159.2, 145.4, 139.4, 136.2, 132.3, 132.2, 129.5, 128.9, 127.8, 127.7, 127.5, 120.0, 119.8, 110.6, 110.4.



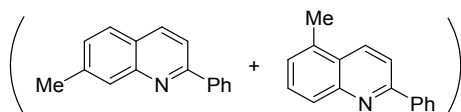
2-phenyl-6-(trifluoromethoxy)quinoline (3ia)¹ White solid. Mp 126-127 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.18 (dd, $J = 21.0, 8.2$ Hz, 4H), 7.93 (d, $J = 8.7$ Hz, 1H), 7.65 (s, 1H), 7.60 – 7.45 (m, 4H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.9, 146.8, 146.5, 139.1, 136.6, 131.9, 129.7, 128.9, 127.6, 127.2, 123.7, 119.9, 117.5.



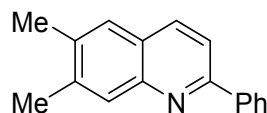
2-phenylquinoline-6-carbonitrile (3ja) ¹ White solid; mp 140-141 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.38 – 8.13 (m, 5), 7.99 (d, *J* = 8.7 Hz, 1), 7.84 (dd, *J* = 8.8, 2.0 Hz, 1), 7.64 – 7.46 (m, 3). ¹³C NMR (101 MHz, CDCl₃) δ 160.0, 149.1, 138.4, 137.1, 133.7, 131.1, 130.4, 130.3, 129.0, 127.8, 126.4, 120.5, 118.7, 109.8.



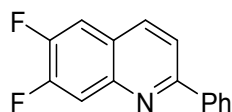
2-phenyl-6-(trifluoromethyl)quinoline (3ka) ¹ White solid. Mp 135 -136 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.22 (dd, *J* = 36.5, 7.8 Hz, 4H), 8.11 (s, 1H), 7.91 (dd, *J* = 27.9, 8.8 Hz, 2H), 7.52 (dt, *J* = 12.1, 6.8 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 159.3, 149.2, 138.8, 137.6, 130.8, 130.0, 129.0, 128.2, 127.9, 127.7, 126.1, 125.5, 125.4, 125.4, 125.4, 122.8, 120.1.



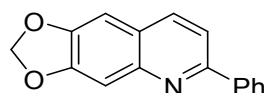
7-methyl-2-phenylquinoline and 5-methyl-2-phenylquinoline mixture (3la / 3la' = 6:1) ¹ White solid. Mp 89-92 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 8.6 Hz, 0.2H), 8.14 (d, *J* = 8.1 Hz, 3.3H), 8.02 (d, *J* = 8.5 Hz, 0.2H), 7.95 (s, 1.0H), 7.87 (d, *J* = 8.9 Hz, 0.2H), 7.79 (d, *J* = 8.4 Hz, 1.0H), 7.69 (d, *J* = 8.1 Hz, 1.0H), 7.62 – 7.56 (m, 0.3H), 7.55 – 7.48 (m, 2.5H), 7.47 – 7.41 (m, 1.3H), 7.34 (d, *J* = 8.3 Hz, 1.2H), 2.69 (s, 0.5H), 2.56 (s, 3.0H). ¹³C NMR (101 MHz, CDCl₃) δ 157.2, 156.8, 148.5, 139.8, 139.8, 139.6, 136.3, 134.3, 133.2, 129.3, 129.2, 129.1, 128.8, 128.7, 128.5, 128.0, 127.5, 127.0, 126.7, 126.4, 125.2, 118.5, 118.1, 21.8, 18.5.



6,7-dimethyl-2-phenylquinoline (3ma) ¹ White solid. Mp 121-122 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.17 (d, *J* = 7.2 Hz, 2H), 8.11 (d, *J* = 2.2 Hz, 1H), 7.98 (s, 1H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.66 – 7.50 (m, 3H), 7.51 – 7.39 (m, 1H), 2.52 (s, 3H), 2.48 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 156.3, 147.3, 139.8, 136.1, 135.6, 128.9, 128.7, 127.4, 126.6, 125.7, 118.1, 20.4, 19.9.

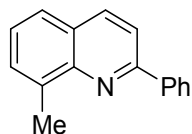


6,7-difluoro-2-phenylquinoline (3na) ¹ White solid. Mp 106-107 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.15 (d, *J* = 7.6 Hz, 3H), 7.94 – 7.87 (m, 2H), 7.57 – 7.49 (m, 4H). ¹³C NMR (101 MHz, CDCl₃) δ 157.6, 153.8, 151.3, 151.1, 148.8, 148.6, 145.4, 145.3, 138.9, 135.9, 135.8, 129.6, 128.8, 127.4, 123.9, 123.8, 119.0, 115.9, 115.7, 112.6, 112.5.

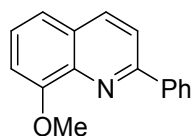


6-phenyl-[1,3]dioxolo[4,5-g]quinoline (3oa) ¹ Light yellow solid. Mp 111-112 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.10 (d, *J* = 7.6 Hz, 2H), 8.02 (d, *J* = 8.3 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.55 – 7.36 (m, 4H), 7.06 (s, 1H), 6.11 (s, 2H).

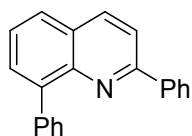
^{13}C NMR (101 MHz, CDCl_3) δ 155.1, 150.8, 147.6, 146.3, 139.5, 135.5, 128.8, 128.6, 127.2, 124.0, 117.1, 106.0, 102.4, 101.6.



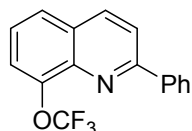
8-methyl-2-phenylquinoline (3pa)¹ Light yellow solid. Mp 46-47 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.25 (d, J = 7.2 Hz, 2H), 8.17 (d, J = 8.5 Hz, 1H), 7.89 (d, J = 8.6 Hz, 1H), 7.65 (d, J = 8.2 Hz, 1H), 7.60 – 7.48 (m, 3H), 7.48 – 7.36 (m, 2H), 2.90 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.5, 147.1, 139.8, 137.7, 136.9, 129.7, 129.2, 128.8, 127.5, 127.1, 126.0, 125.4, 118.2, 17.9.



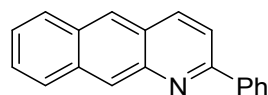
8-methoxy-2-phenylquinoline (3qa)¹ Light yellow solid. Mp 55-56 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.24 – 8.14 (m, 3H), 7.91 (d, J = 8.7 Hz, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.47 – 7.39 (m, 3H), 7.08 (d, J = 7.4 Hz, 1H), 4.12 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 156.2, 155.5, 140.1, 139.7, 136.8, 129.2, 128.7, 128.3, 127.7, 126.5, 119.5, 119.3, 108.1, 56.1.



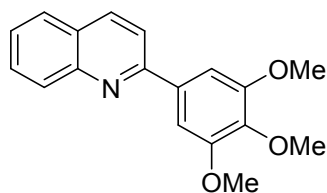
2,8-diphenylquinoline (3ra)¹ yellow oil, ^1H NMR (400 MHz, CDCl_3) δ 8.23 (d, J = 8.5 Hz, 1H), 8.16 (d, J = 7.5 Hz, 2H), 7.94 (dd, J = 8.7, 2.3 Hz, 1H), 7.86 (d, J = 7.7 Hz, 2H), 7.79 (t, J = 7.7 Hz, 2H), 7.65 – 7.34 (m, 7H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.9, 145.5, 140.7, 139.5, 139.4, 137.0, 131.1, 130.4, 129.3, 128.7, 127.6, 127.4, 127.1, 126.1, 118.0.



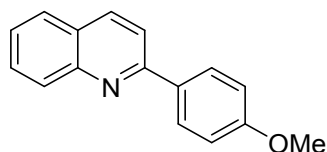
2-phenyl-8-(trifluoromethoxy)quinoline (3sa)¹ White solid. Mp 72-73 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.25 (t, J = 7.4 Hz, 3H), 7.99 (d, J = 8.7 Hz, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.63 (d, J = 7.7 Hz, 1H), 7.52 (dt, J = 15.9, 6.9 Hz, 4H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.5, 145.4, 141.4, 138.9, 136.6, 129.8, 128.8, 128.6, 127.6, 126.4, 125.5, 121.3, 119.5.



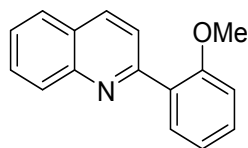
2-phenylbenzo[g]quinoline (3ta)¹ Light yellow solid. Mp 203-204 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.99 (d, J = 8.6 Hz, 1H), 8.62 (d, J = 8.1 Hz, 1H), 8.21 (d, J = 7.7 Hz, 2H), 8.09 (d, J = 9.1 Hz, 1H), 8.01 (t, J = 8.3 Hz, 2H), 7.94 (d, J = 7.8 Hz, 1H), 7.67 (dt, J = 22.4, 7.3 Hz, 2H), 7.54 (t, J = 7.5 Hz, 2H), 7.46 (t, J = 7.3 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 156.9, 148.2, 139.4, 131.7, 131.6, 131.0, 129.6, 129.3, 128.9, 128.7, 128.6, 127.5, 127.1, 127.1, 124.2, 122.6, 118.8.



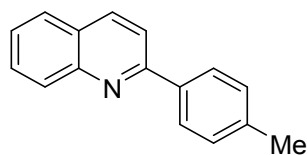
2-(3,4,5-trimethoxyphenyl)quinoline (3ab)¹ Light yellow solid. Mp 150-151 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.25 – 8.13 (m, 2H), 7.90 – 7.80 (m, 2H), 7.77 – 7.68 (m, 1H), 7.60 – 7.47 (m, 1H), 7.40 (d, *J* = 2.4 Hz, 2H), 4.00 (s, 6H), 3.92 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 157.0, 153.6, 148.1, 139.5, 136.8, 135.3, 129.8, 129.6, 127.5, 127.1, 126.3, 118.9, 105.0, 61.0, 56.3.



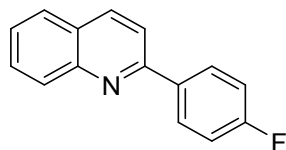
2-(4-methoxyphenyl)quinoline (3ac)² White solid. Mp 119-120°C; ¹H NMR (400 MHz, CDCl₃) δ 8.06 – 7.94 (m, 4H), 7.71 – 7.60 (m, 2H), 7.56 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.34 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 6.97 – 6.85 (m, 2H), 3.71 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.9, 156.9, 148.3, 136.6, 132.3, 129.6, 129.5, 128.9, 127.5, 126.9, 125.9, 118.5, 114.3, 55.4.



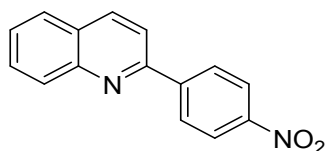
2-(2-methoxyphenyl)quinoline (3ad)² Yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 8.15 (dd, *J* = 16.8, 8.5 Hz, 2H), 7.94 – 7.78 (m, 3H), 7.70 (td, *J* = 7.5, 6.9, 1.5 Hz, 1H), 7.59 – 7.48 (m, 1H), 7.45 – 7.37 (m, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 7.03 (d, *J* = 8.3 Hz, 1H), 3.85 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 157.2, 157.1, 148.3, 135.1, 131.5, 130.3, 129.7, 129.6, 129.2, 127.3, 127.0, 126.1, 123.4, 121.3, 111.5, 55.6.



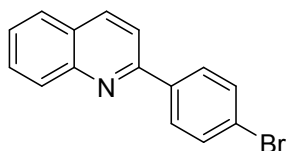
2-(p-tolyl)quinoline (3ae)² White solid. mp 80-81 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.05 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.02 – 7.90 (m, 3H), 7.72 – 7.60 (m, 2H), 7.57 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.35 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.19 (d, *J* = 7.9 Hz, 2H), 2.29 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 157.3, 148.4, 139.4, 136.9, 136.7, 129.7, 129.6, 127.5, 127.2, 126.1, 118.8, 21.4.



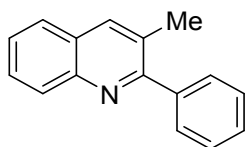
2-(4-fluorophenyl)quinoline (3af)² White solid. Mp 95-96 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.23 – 8.07 (m, 4H), 7.77 (td, *J* = 5.5, 2.8 Hz, 2H), 7.70 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.49 (ddd, *J* = 8.0, 6.7, 1.1 Hz, 1H), 7.22 – 7.00 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 165.1, 162.6, 156.2, 148.2, 136.9, 135.8, 135.8, 129.8, 129.6, 129.5, 129.4, 127.5, 127.1, 126.4, 118.6, 115.9, 115.7, 77.4, 77.1, 76.8



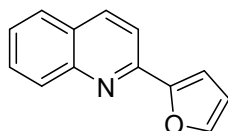
2-(4-nitrophenyl)quinoline (3ag)¹ Yellow solid. Mp 141-142 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.31 (d, *J* = 1.8 Hz, 4H), 8.25 (d, *J* = 8.7 Hz, 1H), 8.17 (d, *J* = 8.6 Hz, 1H), 7.92 – 7.81 (m, 2H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 154.4, 148.3, 148.2, 145.4, 137.3, 130.2, 129.9, 128.2, 127.5, 127.3, 124.0, 118.7.



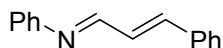
2-(4-bromophenyl)quinoline (3ah)² White solid. Mp 120-121 °C ¹H NMR (400 MHz, CDCl₃) δ 8.17 (dd, *J* = 14.6, 8.6 Hz, 2H), 8.07 – 7.97 (m, 2H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.72 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.52 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 156.0, 148.2, 138.4, 137.0, 132.0, 129.9, 129.7, 129.1, 127.5, 127.3, 126.5, 124.0, 118.5.



3-methyl-2-phenylquinoline (3ai)² Yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.99 (s, 1H), 7.76 (d, *J* = 8.3 Hz, 1H), 7.69 – 7.61 (m, 1H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.54 – 7.41 (m, 4H), 2.45 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.6, 146.7, 141.0, 136.8, 129.4, 129.3, 128.9, 128.8, 128.4, 128.3, 128.2, 127.7, 126.8, 126.5, 20.7.



2-(furan-2-yl)quinoline (3aj)³ White solid. Mp 90-91 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.15 (d, *J* = 8.6 Hz, 2H), 7.81 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.70 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.49 (ddd, *J* = 8.0, 6.9, 1.1 Hz, 1H), 7.26 (s, 1H), 6.59 (dd, *J* = 3.4, 1.7 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 153.5, 148.9, 147.9, 144.2, 136.8, 123.0, 129.2, 127.6, 127.1, 126.3, 117.5, 112.3, 110.4.



N-cinnamylideneaniline ¹H NMR (400 MHz, CDCl₃) δ 8.30 (dd, *J* = 5.2, 3.1 Hz, 1H), 7.66 – 7.48 (m, 2H), 7.48 – 7.34 (m, 5H), 7.32 – 7.22 (m, 3H), 7.20 – 7.12 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 161.6, 151.8, 144.0, 135.7, 129.6, 129.2, 129.0, 128.6, 127.6, 126.2, 121.0.

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