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A Novel Approach for the One-Pot Preparation of α-Amino Amides by Pd-Catalyzed Double Carbohydroamination

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Selected physical data for α-amino amides **2** and **5** (^{1}H and ^{13}C NMR, MS, IR, and elemental analysis) are given as follows:

2a: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 7.49 (d br., J = 8.4 Hz, 1H, NH), 7.29 (m, 5H, Ph), 4.22 (s, 1H, C*H*(CO)), 3.76 (m, 1H, CONHC*H*), 2.41 (m, 1H, CHNHC*H*), 1.89-0.98 (m, 20H, 2Cy); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 171.7 (CO), 140.5 (C_{quat}), 128.7 (CH), 127.8 (CH), 127.1 (CH), 65.3 (CH), 56.4 (CH), 47.4 (CH), 34.2 (CH_2), 33.6 (CH_2), 33.1 (CH_2), 32.9 (CH_2), 25.9 (CH_2), 25.5 (CH_2), 25.1 (CH_2), 25.0 (CH_2), 24.7 (CH_2), 24.6 (CH_2); MS (4 kV needle, ESI), m/z: 315 [M^+ + 1]; IR (KBr): v = 1644 cm^{-1} (C=O); elemental analysis (%) calcd or $C_{20}H_{30}N_2O$: C 76.39, H 9.62, N 8.91; found: C 76.73, H 9.91, N 8.70.

2b: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 7.4-7.2 (m, 6H, Ph and NH), 4.10 (s, 1H, C*H*(CO)), 3.23 (m, 2H, CONHCH_2), 2.59 (m, 2H, CHNHCH_2), 1.6-1.2 (m, 8H, 2(CH_2)$_2$CH_3), 0.89 (t, J = 7.1 Hz, 6H, 2CH_3); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 172.0 (CO), 139.7 (C_{quat}), 128.7 (CH), 127.9 (CH), 127.1 (CH), 67.9 (CH), 48.5 (CH_2), 38.7 (CH_2), 32.2 (CH_2), 31.6 (CH_2), 20.3 (CH_2), 20.0 (CH_2), 13.8

(CH_3), 13.6(CH_3); MS (4 kV needle, ESI), m/z: 263 [M^+ + 1]; IR (KBr): v = 1651 cm^{-1} (C=O).

2c: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 7.4-7.1 (m, 16H, 3Ph and NH), 4.47 (s, 1H, C*H*(CO)), 4.41 (d, J = 6.1 Hz, 2H, CONHC*H*$_2$), 3.77 (s, 2H, CHNHC*H*$_2$); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 170.9 (CO), 139.4 (C_{quat}), 138.1 (C_{quat}), 137.5 (C_{quat}), 129-127 (m, CH), 66.1 (CH), 51.7 (CH_2), 43.3 (CH_2); MS (4 kV needle, ESI), m/z: 331 [M^+ + 1]; IR (KBr): v = 1652 cm^{-1} (C=O).

5a: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 7.49 (d br., J = 8.4 Hz, 1H, NH), 7.20 (d, J = 8.0 Hz, 2H, Ph), 7.09 (d, J = 8.0 Hz, 2H, Ph), 4.21 (s, 1H, C*H*(CO)), 3.73 (m, 1H, CONHC*H*), 2.38 (m, 1H, CHNHC*H*), 2.29 (s, 3H, CH_3), 2.0-1.0 (m, 20H, 2Cy); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 171.9 (CO), 137.5 (C_{quat}), 137.4 (C_{quat}), 129.4 (CH), 127.0 (CH), 64.9 (CH), 56.3 (CH), 47.4 (CH), 34.1 (CH_2), 33.6 (CH_2), 33.0 (CH_2), 32.9 (CH_2), 25.9 (CH_2), 25.5 (CH_2), 25.1 (CH_2), 25.0 (CH_2), 24.7 (CH_2), 24.6 (CH_2), 21.0(CH_3); MS (4 kV needle, ESI), m/z: 329 [M^+ + 1]; IR (KBr): v = 1645 cm^{-1} (C=O); elemental analysis (%) calcd or $C_{21}H_{32}N_2O$: C 76.78, H 9.82, N 8.53; found: C 76.93, H 9.68, N 8.62.

5b: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 7.51 (d br., J = 8.4 Hz, 1H, NH), 7.24 (d, J = 8.6 Hz, 2H, Ph), 6.81 (d, J = 8.6 Hz, 2H, Ph), 4.22 (s, 1H, C*H*(CO)), 3.75 (s, 3H, CH_3), 3.71 (m, 1H, CONHC*H*, overlapped with the signal of CH_3), 2.39 (m, 1H, CHNHC*H*), 1.95-0.99 (m, 20H, 2Cy); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 171.7 (CO), 159.2 (C_{quat}), 132.4 (C_{quat}), 128.3 (CH), 114.1 (CH), 64.4 (CH), 56.3 (CH), 55.2 (CH), 47.5 (CH_3), 33.9 (CH_2), 33.4 (CH_2), 33.0 (CH_2), 32.9 (CH_2), 25.8

(CH_2), 25.5 (CH_2), 25.0 (CH_2), 24.9 (CH_2), 24.7 (CH_2), 24.6 (CH_2); MS (4 kV needle, ESI), m/z: 345 [M^+ + 1]; IR (KBr): v = 1645 cm^{-1} (C=O); elemental analysis (%) calcd or $C_{21}H_{32}N_2O_2$: C 73.22, H 9.36, N 8.13; found: C 72.97, H 9.49, N 8.04.

5c: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 7.48 (d br., J = 8.5 Hz, 1H, NH), 7.29 (s, 5H, Ph), 4.33 (s, 1H, C*H*(CO)), 3.71 (m, 1H, CONHC*H*), 2.42 (m, 1H, CHNHC*H*), 1.96-1.1 (m, 20H, 2Cy); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 171.0 (CO), 145 (C_{quat}), 133.8 (C_{quat}), 129.0 (CH), 63.9 (CH), 56.3 (CH), 47.8 (CH), 33.2 (CH_2), 32.9 (CH_2), 32.8 (CH_2), 25.6 (CH_2), 25.4 (CH_2), 24.9 (CH_2), 24.8 (CH_2), 24.6 (CH_2); MS (4 kV needle, ESI), m/z: 349 [M^+ + 1]; IR (KBr): v = 1648 cm^{-1} (C=O); elemental analysis (%) calcd or $C_{20}H_{29}ClN_2O$: C 68.85, H 8.38, N 8.03; found: C 68.48, H 8.28, N 7.98.

5d: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 7.56 (d, J = 8.2 Hz, 2H, Ph), 7.5 (1H, NH, overlapped with the signal of Ph), 7.44 (d, J = 8.2 Hz, 2H, Ph), 4.30 (s, 1H, C*H*(CO)), 3.74 (m, 1H, CONHC*H*), 2.41 (m, 1H, CHNHC*H*), 1.88-1.0 (m, 20H, 2Cy); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 171.0 (CO), 144.4 (C_{quat}), 130.0 (q, $^2J_{CF}$ = 32.3 Hz, C_{quat}), 127.5 (CH), 125.7 (q, $^3J_{CF}$ = 3.7 Hz, CH), 124.0 (q, $^1J_{CF}$ = 264 Hz, CF_3), 64.8 (CH), 56.3 (CH), 47.6 (CH), 34.2 (CH_2), 33.7 (CH_2), 33.0 (CH_2), 32.9 (CH_2), 25.8 (CH_2), 25.5 (CH_2), 25.0 (CH_2), 24.9 (CH_2), 24.65 (CH_2), 24.60 (CH_2); MS (4 kV needle, ESI), m/z: 383 [M^+ + 1]; IR (KBr): v = 1645 cm^{-1} (C=O); elemental analysis (%) calcd or $C_{21}H_{29}F_3N_2O$: C 65.95, H 7.64, N 7.32; found: C 66.56, H 7.87, N 7.28.

5e: ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 8.16 (d, J = 8.4 Hz, 1H, Ar), 7.84 (d, J = 8.0 Hz, 1H, Ar), 7.76 (d, J = 8.2 Hz, 1H, Ar), 7.57 (d, J =8.2 Hz, 1H, NH), 7.54-7.38 (m, 4H, Ar), 4.97 (s, 1H, C*H*(CO)), 3.84 (m, 1H, CONHC*H*), 2.60 (m, 1H, CHNHC*H*), 2.0-1.1 (m, 20H, 2Cy); ^{13}C NMR (125.8 MHz, $CDCl_3$, 25 °C): δ = 171.5 (CO), 134-123 (m), 61.7 (CH), 57.2 (CH), 47.7 (CH), 33.6 (CH_2), 33.2 (CH_2), 33.0 (CH_2), 32.9 (CH_2), 25.8 (CH_2), 25.5 (CH_2), 25.0 (CH_2), 24.8 (CH_2), 24.7 (CH_2); MS (4 kV needle, ESI), m/z: 365 [M^+ + 1]; IR (KBr): v = 1644 cm^{-1} (C=O); elemental analysis (%) calcd or $C_{24}H_{32}N_2O$: C 79.08, H 8.85, N 7.68; found: C 78.97, H 9.01, N 7.96.