Supporting Information

Palladium-Catalyzed Selective N-Allylation of Indoles assisted by PEG-Water System

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General consideration

Reagents were obtained from Acros Organics (Geel, Belgium), Tokyo Chemical Industry (Tokyo, Japan), Sigma-Aldrich (St. Louis, USA), and Alfa-Aesar (Ward Hill, MA, USA), and used without further purification. All reactions were carried out under a nitrogen atmosphere. Solvents were dried and distilled by known methods. Column chromatography was performed on silica gel. IR absorption spectra were recorded on Shimadzu IR-27G and Perkin-Elmer System 2000FT-IR spectrophotometers. Proton nuclear magnetic resonance (1H-NMR, 400 MHz) and carbon-13 NMR spectra were measured with Varian Unity-400 spectrometers. Carbon multiplicities were obtained from DEPT experiments. Chemical shifts (δ) and coupling constants (Hz) were measured with respect to TMS or chloroform-d1. Mass and high-resolution mass spectra (HRMS) were taken on a Hewlett-Packard 5989A or JEOL JMS D-100 instrument, with a direct inlet system.

General procedure

A mixture of 1,2,3,4-tetrahydrocarbazole (1a, 1 mmol), allyl acetate (2a, 2 mmol), PEG-6000 (1 g), Pd(OAc)2 (9.7 mg, 0.025 mmol), and (2-Furyl)3P (36.5 mg, 0.05 mmol) in distilled water (5 mL) were refluxed for 2 h. After cooling, the solvent was distilled under reduced pressure. Column chromatography (n-hexane/EtOAc = 4:1) of the residue only afforded 143 mg (68%) of 3a and 40 mg (19%) of 4a, respectively.

Products 3a1, 4a1, 3b1, 4b1, 3c1, 4c1, 3d2, 3e3, 3f1, 3g1, 3h4, 3i1 and 3j1 are known.
Characterization data of compound

3a: N-allyl-1,2,3,4-tetrahydrocarbazole

Yellow oil. IR (KBr): ν 1644, 1613, 1464 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.47 (d, J = 7.6 Hz, 1H, ArH), 7.22 (d, J = 8.4 Hz, 1H, ArH), 7.12 (ddd, J = 8.4, 6.8, 0.8 Hz, 1H, ArH), 7.06 (ddd, J = 8.4, 6.8, 0.8 Hz, 1H, ArH), 5.90 (ddt, J = 17.2, 10.4, 4.8 Hz, 1H, vinyl H), 5.09 (ddt, J = 10.4, 1.6, 1.6 Hz, 1H, vinyl H), 4.88 (ddt, J = 17.2, 1.6, 1.6 Hz, 1H, vinyl H), 4.62 (dt, J = 4.8, 1.6 Hz, 2H, NCH₂), 5.09 (ddt, J = 10.4, 1.6, 1.6 Hz, 1H, vinyl H), 4.88 (dt, J = 4.8, 1.6 Hz, 2H, NCH₂), 2.73 (tt, J = 6.0, 1.6 Hz, 2H, CH₂), 2.67 (tt, J = 6.0, 1.6 Hz, 2H, CH₂), 1.82-1.96 (m, 4H, CH₂ × 2); ¹³C-NMR (100 MHz, CDCl₃): δ 136.2 (C), 135.4 (C), 133.8 (CH), 127.4 (C), 120.5 (CH), 118.7 (CH), 117.7 (CH), 116.0 (CH₂), 109.5 (C), 108.8 (CH), 45.0 (CH₂), 23.2 (CH₂), 23.2 (CH₂), 22.0 (CH₂), 21.1 (CH₂). EI-MS: m/z 211 (M⁺), 196, 183, 168, 154, 142, 128, 115, 89, 77, 63, 51. EI-MS calcd for C₁₅H₁₇N: 211.1361. Found: 211.1363.

4a: N-allyl-1,2,3,4-tetrahydrocarbazole

Yellow oil. IR (KBr): ν 1711, 1641, 1617, 1451 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.58 (d, J = 7.6 Hz, 1H, ArH), 7.31 (dd, J = 7.6, 7.2, 1.2 Hz, 1H, ArH), 7.30 (dd, J = 7.6, 1.2 Hz, 1H, ArH), 7.17 (dd, J = 7.6, 7.2, 1.2 Hz, 1H, ArH), 5.17 (ddt, J = 17.2, 10.0, 6.8 Hz, 1H, vinyl H), 4.94 (ddt, J = 17.2, 2.0, 1.2 Hz, 1H, vinyl H), 4.86 (ddt, J = 10.0, 2.0, 1.2 Hz, 1H, vinyl H), 2.85-2.91 (m, 1H, CH), 2.62 (dt, J = 13.2, 6.4 Hz, 1H, CH), 2.54-2.59 (m, 1H, CH), 2.54 (dt, J = 13.2, 5.6 Hz, 1H, CH) 2.36 (ddt, J = 13.2, 3.2, 2.8 Hz, 1H, CH), 2.18-2.24 (m, 1H, CH), 1.83 (ttq, J = 13.6, 4.0 Hz, 1H, CH), 1.66-1.72 (m, 1H, CH), 1.43 (ttq, J = 13.6, 4.0 Hz, 1H, CH), 1.16 (dt, J = 13.6, 4.0 Hz, 1H, CH); ¹³C-NMR (100 MHz, CDCl₃): δ 188.9 (C), 154.8 (C), 144.6 (C), 132.1 (CH), 127.6 (CH), 124.7 (CH), 121.9 (CH), 120.1 (CH), 118.0 (CH₂), 57.6 (C), 37.6 (CH₂), 37.0 (CH₂), 30.1 (CH₂), 28.8 (CH₂), 21.1 (CH₂). EI-MS: m/z 211 (M⁺), 196, 183, 170, 168, 154, 142, 128, 115, 89, 77, 63, 51. EI-MS calcd for C₁₅H₁₇N: 211.1361. Found: 211.1358.
3b: N- (But-2-en-1-yl)-1, 2, 3, 4-tetrahydrocarbazole

Yellow oil. IR (KBr): ν 1653, 1611, 1462 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.46 (dd, J = 8.0, 1.2 Hz, 1H, ArH), 7.24 (dd, J = 8.0, 1.2 Hz, 1H, ArH), 7.12 (ddd, J = 8.0, 7.2, 1.2 Hz, 1H, ArH), 7.05 (ddd, J = 8.0, 7.2, 1.2 Hz, 1H, ArH), 5.40-5.61 (m, 2H, vinyl H), 4.53-4.55 (m, 2H, NCH₂), 2.73 (tt, J = 6.0, 1.6 Hz, 2H, CH₂), 2.68 (tt, J = 6.0, 1.6 Hz, 2H, CH₂), 1.80-1.95 (m, 4H, CH₂ × 2), 1.63 (dd, J = 6.4, 1.2 Hz, 3H, CH₃); ¹³C-NMR (100 MHz, CDCl₃): δ 136.0 (C), 135.3 (C), 127.3 (C), 126.7 (CH), 120.4 (CH), 118.6 (CH), 117.7 (CH), 109.3 (C), 108.9 (CH), 44.4 (CH₂), 23.3 (CH₂), 23.2 (CH₂), 22.1 (CH₂), 21.1 (CH₂), 17.5 (CH₃). EI-MS: m/z 225 (M⁺), 210, 197, 182, 168, 154, 143, 128, 115, 89, 77, 63, 51. EI-HRMS calcd for C₁₆H₁₉N: 225.1517. Found: 225.1517.

4b: 4a-(But-2-en-1-yl)-2,3,4,4a-tetrahydro-1H-carbazole

Yellow oil. IR (KBr): ν 1711, 1616, 1584, 1450 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.57 (d, J = 7.6 Hz, 1H, ArH), 7.26-7.34 (m, 2H, ArH), 7.17 (t, J = 7.6 Hz, 1H, ArH), 5.37 (dq, J = 13.6, 6.4 Hz, 1H, vinyl H), 4.83 (tq, J = 13.6, 6.4 Hz, 1H, vinyl H), 2.84-2.89 (m, 1H, CH), 2.55-2.61 (m, 1H, CH) 2.54 (dt, J = 13.6, 5.6 Hz, 1H, CH) 2.44 (dd, J = 13.6, 7.6 Hz, 1H, CH) 2.34 (dq, J = 13.6, 2.8 Hz, 1H, CH), 2.15-2.24 (m, 1H, CH), 1.81 (tq, J = 13.6, 4.0 Hz, 1H, CH), 1.64-1.69 (m, 1H, CH), 1.48 (dd, J = 6.4, 0.8 Hz, 3H, CH₃), 1.41 (tq, J = 13.6, 4.0 Hz, 1H, CH), 1.12 (dt, J = 13.6, 4.0 Hz, 1H, CH); ¹³C-NMR (100 MHz, CDCl₃): δ 189.2 (C), 154.8 (C), 144.9 (C), 128.6 (CH), 127.4 (CH), 124.5 (CH), 124.4 (CH), 121.9 (CH), 120.0 (CH), 57.8 (C), 36.7 (CH₂), 36.4 (CH₂), 30.1 (CH₂), 28.8 (CH₂), 21.0 (CH₂), 17.7 (CH₃). EI-MS: m/z 225 (M⁺), 210, 196, 182, 168, 154, 143, 128, 115, 89, 77, 63. EI-HRMS calcd for C₁₆H₁₉N: 225.1517. Found: 225.1518.
3c: N-(Hex-2-en-1-yl) -1, 2, 3, 4-tetrahydrocarbazole

Yellow oil. IR (KBr): v 1658, 1613, 1464 cm\(^{-1}\). \(^1\)H-NMR (400 MHz, CDCl\(_3\)): \(\delta 7.54 (d, J = 7.6 \text{ Hz}, 1 \text{H, ArH}), 7.32 (d, J = 8.0 \text{ Hz}, 1 \text{H, ArH}), 7.20 (dt, J = 8.0, 1.2 \text{ Hz}, 1 \text{H, ArH}), 7.13 (dt, J = 7.6, 1.2 \text{ Hz}, 1 \text{H, ArH}), 5.47-5.61 (m, 2H, vinyl H), 4.63 (dd, J = 4.8, 1.2 Hz, 2H, NCH\(_2\)), 2.81 (t, J = 6.0 Hz, 2H, CH\(_2\)), 2.75 (t, J = 6.0 Hz, 2H, CH\(_2\)), 1.90-2.05 (m, 6H, CH\(_2\) x 3), 1.41 (hext, J = 7.6 Hz, 2H, CH\(_2\)), 0.92 (t, J = 7.6 Hz, 3H, CH\(_3\)) ; \(^{13}\)C-NMR (100 MHz, CDCl\(_3\)): \(\delta 136.1 (C), 135.3 (C), 132.6 (CH), 127.3 (C), 125.6 (CH), 120.4 (CH), 118.5 (CH), 117.6 (CH), 109.3 (C), 108.9 (CH), 44.6 (CH\(_2\)), 36.5 (CH\(_2\)), 23.3 (CH\(_2\)), 23.2 (CH\(_2\)), 22.2 (CH\(_2\)), 22.1 (CH\(_2\)), 21.1 (CH\(_2\)), 13.6 (CH\(_3\)).\) EI-MS: \(m/z\) 253 (M\(^+\)), 225, 210, 196, 182, 168, 154, 143, 128, 115, 89, 77, 63, 55. EI-HRMS calcd for C\(_{18}\)H\(_{23}\)N: 253.1830. Found: 253.1830.

4c: 4a-(Hex-2-en-1-yl)-2,3,4,4a-tetrahydro-1\(H\)-carbazole

Yellow oil. IR (KBr): v 1711, 1616, 1586, 1463 cm\(^{-1}\). \(^1\)H-NMR (400 MHz, CDCl\(_3\)): \(\delta 7.57 (d, J = 7.6 \text{ Hz}, 1 \text{H, ArH}), 7.31 (dt, J = 7.6, 1.2 \text{ Hz}, 1 \text{H, ArH}), 7.28 (dd, J = 7.6, 1.2 \text{ Hz}, 1 \text{H, ArH}), 7.17 (dt, J = 7.6, 1.2 \text{ Hz}, 1 \text{H, ArH}), 5.33 (dt, J = 15.2, 6.8 Hz, 1H, vinyl H), 4.81 (dt, J = 15.2, 6.8 Hz, 1H, vinyl H), 2.85-2.90 (m, 1H, CH), 2.53-2.59 (m, 2H, CH\(_2\)), 2.49 (dt, J = 13.6, 7.6 Hz, 1H, CH), 2.35 (dq, J = 13.6, 2.8 Hz, 1H, CH), 2.16-2.23 (m, 1H, CH), 1.65-1.88 (m, 4H, CH x 4), 1.43 (tq, J = 13.6, 4.4 Hz, 1H, CH), 1.15-1.23 (m, 2H, CH\(_2\)), 1.14 (dt, J = 13.6, 4.4 Hz, 1H, CH), 0.73 (t, J = 7.2, Hz, 3H, CH\(_3\)); \(^{13}\)C-NMR (100 MHz, CDCl\(_3\)): \(\delta 189.2 (C), 154.8 (C), 144.9 (C), 134.2 (CH), 127.4 (CH), 124.5 (CH), 123.3 (CH), 121.9 (CH), 120.0 (CH), 57.9 (C), 36.7 (CH\(_2\)), 36.4 (CH\(_2\)), 34.3 (CH\(_2\)), 30.1 (CH\(_2\)), 28.8 (CH\(_2\)), 22.4 (CH\(_2\)), 21.1 (CH\(_2\)), 13.4 (CH\(_3\)).\) EI-MS: \(m/z\) 253 (M\(^+\)), 225, 210, 196, 182, 168, 154, 143, 128, 115, 89, 77, 63, 55. EI-HRMS calcd for C\(_{18}\)H\(_{23}\)N: 253.1830. Found: 253.1832.
3d: N-(2-Methylallyl)-tetrahydrocarbazole

Deep brown oil. IR (KBr): ν 1656, 1614, 1465 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.50 (d, J = 7.2 Hz, 1H, ArH), 7.24 (d, J = 8.4 Hz, 1H, ArH), 7.15 (ddd, J = 8.4, 6.8, 1.2 Hz, 1H, ArH), 7.09 (ddd, J = 7.2, 6.8, 1.2 Hz, 1H, ArH), 4.84 (dq, J = 3.2, 0.8 Hz, 1H, vinyl H), 4.54 (s, 2H, NCH₂), 4.50 (s, 1H, vinyl H), 2.60 (tt, J = 6.0, 1.2 Hz, 2H, CH₂), 2.60 (tt, J = 6.0, 1.2 Hz, 2H, CH₂) 1.80-1.96 (m, 4H, CH₂ x 2), 1.72 (s, 3H, CH₃); ¹³C-NMR (100 MHz, CDCl₃): δ 141.4 (C), 136.5 (C), 135.6 (C), 127.3 (C), 120.5 (CH), 118.6 (CH), 117.6 (CH), 111.7 (CH), 111.2 (CH), 109.4 (C), 108.9 (CH), 48.5 (CH₂), 23.2 (CH₂), 23.2 (CH₂), 22.0 (CH₂), 21.1 (CH₂), 20.0. (CH₃). EI-MS: m/z 225 (M⁺), 210, 197, 182, 168, 142, 115, 89, 77, 44. EI-HRMS calcd for C₁₆H₁₉N: 225.1517. Found: 225.1517.

3e: 9-(3-methylbut-2-en-1-yl)-2,3,4,9-tetrahydro-1H-carbazole

Deep brown oil. IR (KBr): ν 1678, 1654, 1612, 1463 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.47 (d, J = 7.6 Hz, 1H, ArH), 7.24 (d, J = 8.0 Hz, 1H, ArH), 7.13 (dt, J = 8.0, 1.2 Hz, 1H, ArH), 7.06 (ddd, J = 8.0, 7.6, 1.2 Hz, 1H, ArH), 5.17-5.21 (m, 1H, vinyl H), 4.62 (d, J = 6.8 Hz, 2H, NCH₂), 2.73 (tt, J = 6.4, 1.6 Hz, 2H CH₂), 2.70 (tt, J = 6.4, 1.6 Hz, 2H CH₂), 1.85-1.97 (m, 4H, CH₂ x 2), 1.84 (s, 3H, CH₃), 1.70 (s, 3H, CH₃); ¹³C-NMR (100 MHz, CDCl₃): δ 135.2 (C), 133.9 (C), 127.3 (C), 125.5 (C), 121.1 (CH), 120.3 (CH), 118.5 (CH), 117.7 (CH), 109.3 (C), 108.8 (CH), 40.9 (CH₂), 25.5 (CH₂), 23.3 (CH₂), 23.2 (CH₂), 22.2 (CH₂), 21.1 (CH₃), 18.0 (CH₃). EI-MS: m/z 239 (M⁺), 211, 196, 183, 171, 168, 115, 89, 77. EI-HRMS calcd for C₁₇H₂₁N: 239.1674. Found: 239.1677.

3f: N-Allyl-3-methylindole
Yellow oil. IR (KBr): ν 1614, 1459 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.57 (ddd, J = 8.4, 1.2, 0.8 Hz, 1H, ArH), 7.27 (ddd, J = 8.0, 1.2, 0.8 Hz, 1H, ArH), 7.18 (ddd, J = 8.4, 6.8, 1.2 Hz, 1H, ArH), 7.10 (ddd, J = 8.0, 6.8, 0.8 Hz, 1H, ArH), 6.86 (s, J = 1 Hz, ArH), 5.96 (ddt, J = 17.2, 10.0, 5.2 Hz, 1H, vinyl H), 5.16 (ddt, J = 10.0, 1.6, 1.2 Hz, 1H, vinyl H), 5.07 (ddt, J = 17.2, 1.6, 1.2 Hz, 1H, vinyl H), 4.65 (dt, J = 5.2, 1.6 Hz, 2H, NCH₂), 2.32 (s, 3H, CH₃); ¹³C-NMR (100 MHz, CDCl₃): δ 136.4 (C), 133.8 (CH), 128.9 (C), 125.4 (CH), 121.4 (CH), 119.0 (CH), 118.6 (CH), 117.0 (CH₂), 110.5 (C), 109.3 (CH), 48.5 (CH₂), 9.6 (CH₃). EI-MS: m/z 171 (M⁺), 156, 144, 139, 103, 87, 77, 51. EI-HRMS calcd for C₁₂H₁₃N: 171.1048. Found: 171.1051.

3g: N-allyl-2,3-dimethylindole

Yellow oil. IR (KBr): ν 1696, 1614, 1452 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.49 (dd, J = 7.6, 1.2 Hz, 1H, ArH), 7.20 (ddd, J = 7.6, 7.2, 1.2 Hz, 1H, ArH), 7.12 (ddd, J = 7.6, 7.2, 1.2 Hz, 1H, ArH), 7.07 (ddd, J = 7.6, 7.2, 1.2 Hz, 1H, ArH), 5.92 (ddt, J = 17.2, 10.4, 4.4 Hz, 1H, vinyl H), 5.09 (ddt, J = 10.4, 2.0, 1.2 Hz, 1H, vinyl H), 4.82 (ddt, J = 17.2, 2.0, 1.2 Hz, 1H, vinyl H), 4.66 (dt, J = 4.4, 2.0 Hz, 2H, CH₂), 2.31 (s, 3H, CH₃), 2.26 (s, 3H, CH₃); ¹³C-NMR (100 MHz, CDCl₃): δ 136.0 (C), 133.7 (CH), 132.2 (C), 128.5 (C), 120.5 (CH), 118.7 (CH), 117.9 (CH), 115.9 (CH₂), 108.6 (CH), 106.7 (C), 45.3 (CH₂), 9.9 (CH₃), 8.8 (CH₃). EI-MS: m/z 185 (M⁺), 170, 158, 144, 128, 115, 102, 88, 77, 51. EI-HRMS calcd for C₁₃H₁₅N: 185.1204. Found: 185.1202.

3h: 3-Allyl-1,2-dimethyl-3H-benzo[e]indole

Yellow oil. IR (KBr): ν 1647, 1592, 1441 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 8.59 (d, J = 8.4 Hz, 1H, ArH), 7.96 (d, J = 8.0 Hz, 1H, ArH), 7.58 (d, J = 8.8 Hz, 1H, ArH), 7.58 (ddd, J = 8.4, 6.8, 1.2 Hz, 1H, ArH), 7.45 (d, J = 8.8 Hz, 1H, ArH), 7.43 (ddd, J = 8.0, 6.8, 1.2 Hz, 1H, ArH), 5.99 (ddt, J = 17.2, 10.4, 4.4 Hz, 1H, vinyl H), 5.14 (ddt, J = 10.4, 1.6, 1.2 Hz, 1H, vinyl H), 4.80 (dt, J = 4.4, 1.6 Hz, 2H, NCH₂), 4.76 (ddt, J = 17.2, 1.6, 1.2 Hz, 2H, vinyl H), 2.73 (s, 3H, CH₃), 2.43 (s, 3H, CH₃); ¹³C-NMR (100 MHz, CDCl₃): δ 133.6 (CH), 132.3 (C), 130.6 (C), 129.2 (C), 128.6 (CH), 125.1 (CH), 123.2 (CH), 122.3 (CH), 121.4 (CH), 121.0 (C), 116.0 (CH₂), 110.8 (CH), 109.3 (C), 45.4 (CH₂), 12.8 (CH₃), 9.7 (CH₃). EI-MS: m/z 235 (M⁺), 220, 194, 178, 152, 127, 108, 75. EI-HRMS calcd for C₁₇H₁₇N: 235.1361. Found: 235.1359.
3i: 4-allyl-1,2,3,4-tetrahydrocyclopenta[b]indole

Yellow oil. IR (KBr): ν 1650, 1610, 1457 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.47 (dd, J = 7.2, 0.8 Hz, 1H, ArH), 7.26 (dd, J = 7.2, 1.6 Hz, 1H, ArH), 7.13 (dt, J = 7.2, 1.6 Hz, 1H, ArH), 7.08 (dt, J = 7.2, 0.8 Hz, 1H, ArH), 5.97 (ddt, J = 16.0, 10.4, 5.2 Hz, 1H, vinyl H), 5.16 (ddt, J = 10.4, 1.6, 1.6 Hz, 1H, vinyl H), 5.03 (ddt, J = 16.0, 1.6, 1.6 Hz, 1H, vinyl H), 4.66 (dt, J = 5.2, 1.6 Hz, 2H, NCH₂), 2.89 (t, J = 7.2 Hz, 2H, CH₂), 2.85 (t, J = 6.0 Hz, 2H, CH₂), 2.56 (quin, J = 6.8 Hz, 2H, CH₂); ¹³C-NMR (100 MHz, CDCl₃): δ 146.1 (C), 140.8 (C), 133.7 (CH), 124.5 (C), 119.9 (CH), 119.0 (CH), 118.5. (CH), 118.0 (C), 116.4 (CH₂), 109.7 (CH), 47.1 (CH₂), 28.4 (CH₂), 25.0 (CH₂), 24.6 (CH₂). EI-MS: m/z 197 (M⁺), 182, 168, 154, 143, 128, 115, 77. EI-HRMS calcd for C₁₄H₁₅N: 197.1204. Found: 197.1202.

3j: N-allyl-6,7,8,9,10,10a-hexahydro-cyclohepta[b]indole

Yellow oil. IR (KBr): ν 1643, 1611, 1465 cm⁻¹. ¹H-NMR (400 MHz, CDCl₃): δ 7.56 (dd, J = 7.6 Hz, 1.2, 1H, ArH), 7.25 (dd, J = 7.2, 1.2 Hz, 1H, ArH), 7.17 (dt, J = 7.2, 1.2 Hz, 1H, ArH), 7.13 (dt, J = 7.2, 1.2 Hz, 1H, ArH), 5.97 (ddt, J = 17.2, 10.4, 4.4 Hz, 1H, vinyl H), 5.14 (ddt, J = 10.4, 2.0, 1.2 Hz, 1H, vinyl H), 4.88 (ddt, J = 17.2, 2.0, 1.2 Hz, 1H, vinyl H), 4.73 (dt, J = 4.4, 2.0 Hz, 2H, NCH₂), 2.84-2.93 (m, 4H, CH₂×2), 1.80-1.98 (m, 6H, CH₂×3); ¹³C-NMR (100 MHz, CDCl₃): δ 138.8 (C), 135.3 (C), 134.0 (CH), 127.9 (C), 120.3 (CH), 118.7 (CH), 117.6 (CH), 115.8 (CH₂), 113.9 (C), 108.8 (CH), 45.0 (CH₂), 31.7 (CH₂), 28.4 (CH₂), 27.2 (CH₂), 26.3 (CH₂) 24.4 (CH₂). EI-MS: m/z 225 (M⁺), 209, 196, 182, 168, 156, 142, 128, 115, 89, 77, 63, 51. EI-HRMS calcd for C₁₆H₁₉N: 225.1517. Found: 225.1517.
$^1$H and $^{13}$C NMR spectra of 3a
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$^1$H and $^{13}$C NMR spectra of 3b
$^1$H and $^{13}$C NMR spectra of 4b
$^1$H and $^{13}$C NMR spectra of 3c
$^1$H and $^{13}$C NMR spectra of 4c
$^1$H and $^{13}$C NMR spectra of 3d
$^1\text{H}$ and $^{13}\text{C}$ NMR spectra of 3e
$^1$H and $^{13}$C NMR spectra of 3f
$^1$H and $^{13}$C NMR spectra of 3g
$^{1}H$ and $^{13}C$ NMR spectra of $3h$
$^1$H and $^{13}$C NMR spectra of 3i
$^1$H and $^{13}$C NMR spectra of 3j
Reference