The N-Aryl Aminocarbonyl *ortho*-Substituent Effect in Cu-Catalyzed Aryl Amination and Its Application in the Synthesis of 5-Substituted 11-Oxo-dibenzodiazepines

Xiaoqiong Diao¹, Lanting Xu¹, Wei Zhu¹, Yongwen Jiang², Haoyang Wang², Yinlong Guo²
and Dawei Ma^{2*}

¹Department of Chemistry, Fudan University, Shanghai 200433, China

²State Key Laboratory of Bioorganic and Natural Products Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Lu, Shanghai 200032, China

Madw@mail.sioc.ac.cn

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Experimental

General procedure for CuCl-catalyzed formation of 11-oxo-dibenzodiazepines from dibromides. A Schlenk tube was charged with dibromides (0.5 mmol), CuCl (5 mg, 0.05 mmol), 1,10-phenanthroline (9 mg, 0.05 mmol), and K₃PO₄ (318 mg, 1.5 mmol). The tube was evacuated and backfilled with argon before amine (0.55 mmol) and 1 mL DMF was added. The reaction mixture was stirred at room temperature for 3-12 h, and then stirred at 50 °C for 12-24 h. After the reaction mixture was diluted with EtOAc and washed with water and brine, the solution was dried over Na₂SO₄, and concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluting with 50:1 petroleum ether/ethyl acetate) to provide the desired product.

5-Benzyl-5H-dibenzo[b,e][1,4]diazepin-11(10H)-one (7a). 135 mg, Yield: 90%. ¹H NMR (400 MHz, CDCl₃) δ 8.93 (s, 1H), 8.14 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.71-7.69 (m, 1H), 7.60-7.57 (m, 1H), 7.43 (d, *J* = 7.5 Hz, 2H), 7.38-7.26 (m, 6H), 6.77-6.72 (m, 2H), 4.66 (d, *J* = 6.0 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 163.51, 149.34, 148.49, 141.93, 139.45, 132.99, 129.20, 128.87 (2C), 127.24, 127.09 (2C), 124.89, 124.48, 119.50, 115.68, 111.75, 110.45, 108.53, 47.22. ESI-HRMS calcd. for C₂₀H₁₇N₂O (M + H)⁺ requires *m/z* 301.1341, found *m/z* 301.1317.

5-Methyl-5H-dibenzo[b,e][1,4]diazepin-11(10H)-one (7b). 82 mg, Yield: 73%. ¹H NMR (400 MHz, CDCl₃) δ 8.25 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.71-7.69 (m, 1H), 7.55-7.54 (m,

1H), 7.39 (t, $J = 7.8$ Hz, 1H), 7.33-7.30 (m, 2H), 6.78 (d, $J = 8.8$ Hz, 1H), 6.74 (t, $J = 7.6$ Hz, 1H), 3.06 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.43, 149.38, 149.19, 141.83, 132.94, 129.01, 124.66, 124.31, 119.22, 115.05, 110.56, 110.26, 108.06, 29.86. ESI-HRMS calcd. for $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}$ ($\text{M} + \text{H}$) $^+$ requires m/z 225.1028, found m/z 225.1038.

5-Propyl-5H-dibenzo[*b,e*][1,4]diazepin-11(10H)-one (7c). 92 mg, Yield: 73%. ^1H NMR (400 MHz, CDCl_3) δ 8.39 (s, 1H), 8.10 (d, $J = 7.2$ Hz, 1H), 7.71-7.69 (m, 1H), 7.57-7.54 (m, 1H), 7.38-7.31 (m, 3H), 6.80 (d, $J = 8.4$ Hz, 1H), 6.72 (t, $J = 7.3$ Hz, 1H), 3.32 (t, $J = 6.4$ Hz, 2H), 1.86 – 1.80 (m, 2H), 1.10 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 163.49, 149.18, 148.66, 141.91, 132.86, 129.12, 124.62, 124.26, 119.30, 114.85, 111.01, 110.24, 107.89, 45.00, 22.58, 11.95. ESI-HRMS calcd. for $\text{C}_{16}\text{H}_{17}\text{N}_2\text{O}$ ($\text{M} + \text{H}$) $^+$ requires m/z 253.1335, found m/z 253.1334.

5-(3-(Dimethylamino)propyl)-5H-dibenzo[*b,e*][1,4]diazepin-11(10H)-one (4). 118 mg, Yield: 80%. ^1H NMR (400 MHz, CDCl_3) δ 8.39 (s, 1H), 8.10 (d, $J = 8.0$ Hz, 1H), 7.70-7.68 (m, 1H), 7.56-7.54 (m, 1H), 7.37-7.31 (m, 3H), 6.81 (d, $J = 8.4$ Hz, 1H), 6.73 (t, $J = 7.5$ Hz, 1H), 3.44 -3.39 (m, 2H), 2.57 (t, $J = 7.4$ Hz, 2H), 2.35 (s, 6H), 2.04-1.98 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.45, 149.19, 148.56, 141.87, 132.90, 129.12, 124.65, 124.30, 119.26, 115.00, 111.05, 110.27, 108.01, 57.53, 45.73 (2C), 41.21, 27.39. ESI-HRMS calcd. for $\text{C}_{18}\text{H}_{22}\text{N}_3\text{O}$ ($\text{M} + \text{H}$) $^+$ requires m/z 296.1757; found m/z 296.1785.

5-(3-Hydroxypropyl)-5H-dibenzo[*b,e*][1,4]diazepin-11(10H)-one (7d). 102 mg, Yield: 76%. ^1H NMR (400 MHz, CDCl_3) δ 8.37 (s, 1H), 8.11 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.71-7.69 (m, 1H), 7.67-7.54 (m, 1H), 7.39-7.31 (m, 3H), 6.84 (d, $J = 8.4$ Hz, 1H), 6.74 (t, $J = 7.4$ Hz, 1H), 3.89 (t, $J = 6.0$ Hz, 2H), 3.50 (t, $J = 6.4$ Hz, 2H), 2.10 – 2.03 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.32, 149.10, 148.43, 141.70, 132.84, 129.09, 124.64, 124.25, 119.23, 115.18, 111.00, 110.19, 108.16, 60.85, 39.96, 32.04. ESI-HRMS calcd. for $\text{C}_{16}\text{H}_{17}\text{N}_2\text{O}_2$ ($\text{M} + \text{H}$) $^+$ requires m/z 269.1290, found m/z 269.1289.

5-Allyl-5H-dibenzo[*b,e*][1,4]diazepin-11(10H)-one (7e). 102 mg, Yield: 82%. ^1H NMR (400 MHz, CDCl_3) δ 8.56 (s, 1H), 8.12 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.73-7.70 (m, 1H), 7.58-7.56 (m, 1H), 7.38-7.31 (m, 3H), 6.80-6.74 (m, 2H), 6.10-6.00 (m, 1H), 5.40 (dd, $J = 17.2, 1.2$ Hz, 1H), 5.24 (dd, $J = 10.4, 1.6$ Hz, 1H), 4.05 (t, $J = 5.2$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.42, 149.24, 148.40, 141.86, 135.01, 132.82, 129.11, 124.74, 124.35, 119.36, 115.97, 115.39, 111.46, 110.31, 108.31, 45.58. ESI-HRMS calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_2\text{O}$ ($\text{M} + \text{H}$) $^+$ requires m/z 251.1184, found m/z 251.1175.

5-(Furan-2-ylmethyl)-5H-dibenzo[*b,e*][1,4]diazepin-11(10H)-one (7f). 99 mg, Yield: 68%. ^1H NMR (400 MHz, CDCl_3) δ 8.80 (s, 1H), 8.12 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.72-7.70 (m, 1H), 7.57-7.55 (m, 1H), 7.40-7.31 (m, 4H), 6.86 (d, $J = 8.4$ Hz, 1H), 6.78 (t, $J = 7.5$ Hz, 1H), 6.35-6.34 (m, 1H), 6.31-6.30 (m, 1H), 4.60 (d, $J = 5.6$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.22, 152.79, 149.20, 148.02, 141.93, 141.74, 132.81, 129.08, 124.77, 124.35, 119.41, 115.87, 111.34, 110.45, 110.29, 108.68, 106.81, 40.67; ESI-HRMS calcd. for $\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}_2\text{Na}$ ($\text{M} + \text{Na}$) $^+$ requires m/z 313.0953; found m/z 313.0948.

5-(2-Morpholinoethyl)-5H-dibenzo[*b,e*][1,4]diazepin-11(10H)-one (7g). 121 mg, Yield: 75%. ^1H NMR (400 MHz, CDCl_3) δ 8.62 (s, 1H), 8.11 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.72-7.69 (m, 1H), 7.57-7.55 (m, 1H), 7.37-7.32 (m, 3H), 6.80-6.73 (m, 2H), 3.83-3.81 (m, 4H), 3.46-3.42 (m, 2H), 2.80 (t, $J = 6.4$ Hz, 2H), 2.60 (s, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.32, 149.27, 148.37, 141.99, 132.90, 129.21, 124.70, 124.34, 119.25, 115.23, 111.19, 110.32, 108.42, 67.35 (2C), 56.95, 53.59 (2C), 40.10. ESI-HRMS calcd. for $\text{C}_{19}\text{H}_{22}\text{N}_3\text{O}_2$ ($\text{M} + \text{H}$) $^+$ requires m/z 324.1707, found m/z 324.1706.

Methyl 6-(11-oxo-10,11-dihydro-5H-dibenzo[b,e][1,4]diazepin-5-yl)hexanoate (7h). 135 mg, Yield: 80%. ^1H NMR (400 MHz, CDCl_3) δ 8.36 (s, 1H), 8.11 (d, $J = 8.0$ Hz, 1H), 7.73-7.71 (m, 1H), 7.56-7.55 (m, 1H), 7.38-7.30 (m, 3H), 6.78 (d, $J = 8.5$ Hz, 1H), 6.73 (t, $J = 7.5$ Hz, 1H), 3.67 (s, 3H), 3.37-3.32 (m, 2H), 2.38 (t, $J = 7.5$ Hz, 2H), 1.87-1.72 (m, 4H), 1.60-1.52 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 174.31, 163.53, 149.26, 148.63, 141.95, 132.98, 129.22, 124.75, 124.39, 119.42, 115.05, 111.05, 110.35, 108.04, 51.74, 43.05, 34.25, 29.06, 27.02, 24.96; ESI-HRMS calcd. for $\text{C}_{20}\text{H}_{23}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}$) $^+$ requires m/z 339.1709; found m/z 339.1695.

5-Benzyl-7-methoxy-5H-dibenzo[b,e][1,4]diazepin-11(10H)-one (7i). 125 mg, Yield: 76%. ^1H NMR (400 MHz, CDCl_3) δ 8.83 (s, 1H), 8.08 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.56 (d, $J = 8.7$ Hz, 1H), 7.42 (d, $J = 7.3$ Hz, 2H), 7.35 (t, $J = 7.5$ Hz, 2H), 7.28-7.24 (m, 2H), 7.12 (d, $J = 2.0$ Hz, 1H), 6.93 (dd, $J = 8.4, 2.4$ Hz, 1H), 6.75-6.69 (m, 2H), 4.64 (d, $J = 5.8$ Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.71, 158.18, 150.24, 148.00, 139.51, 135.67, 132.51, 128.84 (2C), 128.79, 127.20, 127.09 (2C), 119.48, 115.64, 112.46, 111.64, 108.86, 95.50, 56.20, 47.22; ESI-HRMS calcd. for $\text{C}_{21}\text{H}_{18}\text{N}_2\text{NaO}_2$ ($\text{M} + \text{Na}$) $^+$ requires m/z 353.1266, found m/z 353.1251.

5-Allyl-7-methoxy-5H-dibenzo[b,e][1,4]diazepin-11(10H)-one (7j). 112 mg, Yield: 80%.

^1H NMR (400 MHz, CDCl_3) δ 8.47 (s, 1H), 8.07 (d, $J = 7.2$ Hz, 1H), 7.58 (d, $J = 8.8$ Hz, 1H), 7.33 (t, $J = 7.4$ Hz, 1H), 7.11 (d, $J = 2.0$ Hz, 1H), 6.93 (dd, $J = 8.8, 2.0$ Hz, 1H), 6.78-6.73 (m, 2H), 6.09-6.02 (m, 1H), 5.39 (dd, $J = 17.2, 0.9$ Hz, 1H), 5.24 (dd, $J = 10.4, 0.8$ Hz, 1H), 4.03 (s, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (101 MHz, CDCl_3) 162.60, 158.06, 150.10, 147.44, 135.58, 135.05, 132.34, 128.68, 119.32, 115.93, 115.35, 112.31, 111.33, 108.61, 95.40, 56.06, 45.57; ESI-HRMS calcd. for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_2$ ($\text{M} + \text{H}$) $^+$ requires m/z 281.1290, found m/z 281.1288.

5-Benzyl-7-fluoro-5H-dibenzo[b,e][1,4]diazepin-11(10H)-one (7k). 111 mg, Yield: 70%.

^1H NMR (400 MHz, CDCl_3) δ 8.79 (s, 1H), 8.09 (d, $J = 8.0$ Hz, 1H), 7.61 (dd, $J = 8.8, 4.8$ Hz, 1H), 7.43 (d, $J = 7.5$ Hz, 2H), 7.37 (t, $J = 7.5$ Hz, 2H), 7.31-7.27 (m, 3H), 7.08 (dt, $J = 9.2, 2.3$ Hz, 1H), 6.77-6.72 (m, 2H), 4.64 (d, $J = 5.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (100 MHz, CDCl_3) 163.01 (d, $J = 231.3$ Hz), 159.44, 149.35 (d, $J = 14.8$ Hz), 148.29, 139.35, 138.22, 133.08, 129.07, 128.88 (2C), 127.28, 127.10 (2C), 119.61 (d, $J = 10.0$ Hz), 115.75, 112.25 (d, $J = 24.6$ Hz), 111.76, 108.27, 98.62 (d, $J = 28.4$ Hz), 47.23; ESI-HRMS calcd. for $\text{C}_{20}\text{H}_{15}\text{FN}_2\text{NaO}$ ($\text{M} + \text{Na}$) $^+$ requires m/z 341.1066, found m/z 341.1059.

5-Allyl-2-methoxy-5H-dibenzo[b,e][1,4]diazepin-11(10H)-one (7l). 84 mg, Yield: 60%. ^1H NMR (400 MHz, CDCl_3) δ 8.20 (s, 1H), 7.73-7.71 (m, 1H), 7.65 (d, $J = 2.8$ Hz, 1H),

7.58-7.56 (m, 1H), 7.34-7.32 (m, 2H), 7.03 (dd, $J = 9.1, 2.8$ Hz, 1H), 6.75 (d, $J = 9.1$ Hz, 1H), 6.09-6.01 (m, 1H), 5.37 (d, $J = 17.1$ Hz, 1H), 5.22 (d, $J = 10.3$ Hz, 1H), 4.01 (s, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.13, 150.08, 149.20, 143.63, 141.93, 135.41, 124.79, 124.41, 121.28, 119.44, 115.84, 113.02, 112.18, 110.30, 108.07, 56.22, 46.00; ESI-HRMS calcd. for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_2$ ($\text{M} + \text{H}$) $^+$ requires m/z 281.1285, found m/z 281.1285.

2-Fluoro-5-methyl-5H-dibenzo[*b,e*][1,4]diazepin-11(10H)-one (7m). 64 mg, Yield: 53%. ^1H NMR (400 MHz, CDCl_3) δ 8.05 (s, 1H), 7.79 (dd, $J = 9.6, 2.8$ Hz, 1H), 7.72-7.70 (m, 1H), 7.56-7.53 (m, 1H), 7.35-7.33 (m, 2H), 7.13 (dt, $J = 8.8, 2.8$ Hz, 1H), 6.68 (dd, $J = 9.2, 4.4$ Hz, 1H), 3.03 (d, $J = 5.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.82 (d, $J = 233.1$ Hz), 149.28, 146.29, 141.82, 134.53, 125.17, 124.65, 120.35 (d, $J = 22.9$ Hz), 119.55, 114.53 (d, $J = 24.5$ Hz), 111.611 (d, $J = 7.3$ Hz), 110.51, 107.88 (d, $J = 7.7$ Hz), 30.33; ESI-HRMS calcd. for $\text{C}_{14}\text{H}_{12}\text{FN}_2\text{O}$ ($\text{M} + \text{H}$) $^+$ requires m/z 243.0934; found m/z 243.0926.

11-Methyl-6,11-dihydro-5H-benzo[*b*]pyrido[2,3-*e*][1,4]diazepin-5-one (7n). 62 mg, Yield: 55%. ^1H NMR (400 MHz, CDCl_3) δ 8.59 (s, 1H), 8.32 (dd, $J = 4.8, 1.7$ Hz, 1H), 8.26 (dd, $J = 7.7, 1.8$ Hz, 1H), 7.72-7.70 (m, 1H), 7.55-7.53 (m, 1H), 7.36-7.31 (m, 2H), 6.64 (dd, $J = 7.6, 4.8$ Hz, 1H), 3.20 (d, $J = 4.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 161.96, 157.12, 151.84, 149.69, 141.58, 136.82, 125.27, 124.75, 119.66, 111.23, 110.50, 104.54, 28.37; ESI-HRMS calcd. for $\text{C}_{13}\text{H}_{12}\text{N}_3\text{O}$ ($\text{M} + \text{H}$) $^+$ requires m/z 226.0980, found m/z 226.0960.

General procedure for CuCl-catalyzed coupling of 2-halo-*N*-phenyl-benzamides with *N*-nucleophiles. A Schlenk tube was charged with dibromides (1 mmol), CuCl (1 mg, 0.01 mmol) and K₃PO₄ (424 mg, 2 mmol). The tube was evacuated and backfilled with argon before *N*-nucleophile (2 mmol) and 2 mL DMF was added. The reaction mixture was stirred at room temperature for 10-36 h. After EtOAc was added, and the organic layer was washed with water and brine, dried over Na₂SO₄ and concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluting with 10:1 petroleum ether/ethyl acetate) to provide the desired product.

2-(Benzylamino)-*N*-phenylbenzamide (12a). 281 mg, Yield: 93%. ¹H NMR (400 MHz, CDCl₃) δ 7.95 (s, 1H), 7.82 (s, 1H), 7.56 (dd, *J* = 8.6, 1.0 Hz, 2H), 7.51 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.39-7.25 (m, 8H), 7.17-7.14 (m, 1H), 6.70-6.63 (m, 2H), 4.42 (d, *J* = 4.9 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 168.30, 149.90, 139.04, 137.94, 133.39, 129.18 (2C), 128.76 (2C), 127.50, 127.27 (2C), 127.21, 124.64, 120.80 (2C), 115.48, 115.30, 112.51, 47.28; ESI-HRMS calcd. for C₂₀H₁₉N₂O (M + H)⁺ requires *m/z* 303.1497, found *m/z* 303.1498.

***N*-Benzyl-2-(benzylamino)benzamide (12c).** 265 mg, Yield: 84%. ¹H NMR (400 MHz, CDCl₃) δ 8.13 (s, 1H), 7.39-7.29 (m, 10H), 7.27-7.19 (m, 2H), 6.64 (dd, *J* = 8.4, 0.7 Hz, 1H), 6.59-6.55 (m, 1H), 6.35 (s, 1H), 4.60 (d, *J* = 5.6 Hz, 2H), 4.42 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 169.72, 149.62, 139.18, 138.35, 133.01, 128.89 (2C), 128.71 (2C), 127.89 (2C), 127.68, 127.31, 127.21 (2C), 127.11, 115.17, 112.43, 47.30, 43.85; ESI-HRMS calcd. for C₂₀H₂₁N₂O (M + H)⁺ requires *m/z* 317.1654, found *m/z* 317.1622.

2-(Benzylamino)-N-(4-chlorophenyl)benzamide (12d). 286 mg, Yield: 85%. ^1H NMR (400 MHz, CDCl_3) δ 7.89 (s, 1H), 7.80 (s, 1H), 7.44-7.47 (m, 3H), 7.40-7.14 (m, 8H), 6.66 (d, J = 8.4 Hz, 1H), 6.61 (t, J = 7.6 Hz, 1H), 4.38 (d, J = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.22, 149.85, 138.85, 136.46, 133.53, 129.48, 129.06, 128.72, 127.47, 127.20, 121.98, 115.29, 114.99, 112.51, 47.24. ESI-HRMS calcd. for $\text{C}_{20}\text{H}_{17}\text{ClN}_2\text{O}$ ($\text{M}+\text{H}$) $^+$ requires m/z 337.1108, found m/z 337.1081.

2-(Benzylamino)-N-(4-methoxyphenyl)benzamide (12e). 133 mg, Yield: 40%. ^1H NMR (400 MHz, CDCl_3) δ 7.93 (s, 1H), 7.72 (s, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.41 (d, J = 8.8 Hz, 2H), 7.37-7.18 (m, 6H), 6.87 (d, J = 9.2 Hz, 2H), 6.59-6.65 (m, 2H), 4.38 (d, J = 5.2 Hz, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.25, 156.72, 149.76, 139.04, 133.18, 130.82, 128.69, 127.43, 127.24, 127.13, 122.87, 115.48, 115.20, 114.29, 112.36, 55.58, 47.25. ESI-HRMS calcd. for $\text{C}_{21}\text{H}_{20}\text{N}_2\text{O}_2$ ($\text{M}+\text{H}$) $^+$ requires m/z 333.1603, found m/z 333.1597.

2-(Benzylamino)-4-bromo-N-phenylbenzamide (15). 35 mg, Yield: 81% (2,4-dibromo-N-phenylbenzamide: 40 mg, 0.11 mmol). ^1H NMR (400 MHz, CDCl_3) δ 8.00 (t, J = 4.8 Hz, 1H), 7.69 (s, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.30-7.36 (m, 7H), 7.24-7.27 (m, 1H), 7.14 (t, J = 7.6 Hz, 1H), 6.83 (d, J = 1.6 Hz, 1H), 6.75 (dd, J = 1.6, 8.0 Hz, 1H), 4.35 (d, J = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.57, 150.70, 138.07, 137.55, 129.15 (2C), 128.80 (2C), 128.59,

128.09, 127.41, 127.32 (2C), 124.79, 120.78 (2C), 118.14, 115.00, 114.17, 47.21; ESI-MS:
 m/z $[M + H]^+$ 381.2 (^{79}Br), 383.2 (^{81}Br).