Supporting information for

Bu₄NI-Catalyzed Benzylic Acyloxylation of Alkylarenes with Aromatic Aldehydes

Juan Huang, Lan-Tao Li, Hong-Ying Li, Ezizjan Husan, Peng Wang, and Bin Wang*

State Key Laboratory of Medicinal Chemical Biology, College of Pharmacy, Nankai University, 94 Weijin Road, Tianjin 300071, China.

E-mail: wangbin@nankai.edu.cn.

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1. Investigation of Mechanism

a) Control reactions for exploring Cannizaro pathway



Based on these results of Eq. 1S-3S, we think that Cannizaro disproportionation is also possible in this transformation. This pathway has been presented in the main text.

b) Control reactions for exploring radical chain pathway

One would argue that the homolysis of TBPB would lead to benzoyloxy radical and tert-butoxyl radical at high temperature. The thus-generated radicals could abstract a hydrogen atom from benzylic C-H bond to form a benzylic radical, which would react with benzoyloxy radical to give the ester. However, TEMPO did not affect the reaction when TBPB was used instead of benzaldehyde and the desirable ester was obtained in 72% 4S). Furthermore. the yield (Eq. reaction of TBPB with 2-methylquinonline could not occur in the absence of nBu_4NI , even at 100 °C (Eq. 5S). Thus, these results indicate that the radical chain pathway is not possible.

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2. General Information

¹H NMR and ¹³C NMR spectra were recorded on a Bruker AVANCE AV400 (400MHz and 100MHz), unless otherwise noted. Signal positions were recorded in ppm with the abbreviations s, d, t, and m denoting singlet, doublet, triplet, and multiplet respectively. All NMR spectra were recorded in CDCl₃, and chemical shifts were referenced to residual CHCl₃ at 7.26 ppm for ¹H or 77.0 ppm for ¹³C. All coupling constants J were quoted in Hz. Data were reported as follows: chemical shift, multiplicity, coupling constant and integration. High resolution mass spectrometry was conducted using a Varian 7.0 T FTICR-MS or VG ZAB-HS by ESI technique. Reactions were monitored by thin-layer chromatography (TLC) on 0.25mm silica gel glass plates coated with 60 F₂₅₄. Column chromatography was performed on silica gel (200-300 mesh) using a mixture of petroleum ether (60-90°C)/ethyl acetate as eluant. Reactions were carried out under a nitrogen atmosphere. Commercially available reagents were used as received without purification.

3. General Procedure

General procedure for acyloxylation of 2-methyl azaarenes:

To a Schlenk tube charged with *n*-Bu₄NI (73.8 mg, 0.2 mmol, 0.4 equiv) was added aldehyde (1.0 mmol, 2.0 equiv), 2-methylquinoline (0.5 mmol, 1.0 equiv), *t*BuOOH (3.0 mmol, 6.0 equiv), H₂O (4 mL) under N₂ seperately. The mixture was stirred at 80 °C for 12 h. And then the mixture was extracted by ethyl acetate for 3 times. The combined organic phase was concentrated under reduced pressure. And the residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate) to give the products.

General procedure for acyloxylation of alkylarenes:

To a Schlenk tube charged with *n*-Bu₄NI (73.8 mg, 0.2 mmol, 0.2 equiv) was added aldehyde (1.0 mmol, 1.0 equiv), toluene (10 mmol, 10.0 equiv), *t*BuOOH (4.0 mmol, 4.0 equiv), H₂O (2 mL) under N₂ seperately. The mixture was stirred at 80 °C for 17 h. And then the mixture was extracted by ethyl acetate for 3 times. The combined organic phase was concentrated under reduced pressure. And the residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate) to give the products.

4. Characterization Data of Compounds





¹H NMR (400 MHz, CDCl₃): 8.22-8.09 (m, 4H); 7.85-7.82 (m, 1H); 7.77-7.72 (m, 1H); 7.61-7.54 (m, 3H); 7.50-7.45 (m, 2H); 5.67 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.30; 156.40; 147.66; 137.08; 133.28; 130.02; 129.87; 129.18; 128.49; 127.90; 127.66; 127.59; 126.72; 119.41; 67.90;



HRMS[ESI]: calculated for $C_{17}H_{13}NO_2Na$, $[M+Na]^+$: 286.0838, found 286.0835.



3b



¹H NMR (300 MHz, CDCl₃): 8.16-8.13 (m, 3H); 8.01 (d, J = 8.1 Hz, 1H); 7.75 (t, J = 7.2 Hz, 1H); 7.62-7.57 (m, 2H); 7.50-7.42 (m, 3H); 5.65 (s, 2H); 2.74 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 163.40; 152.97; 146.33; 144.95; 132.59; 129.46; 129.14; 128.84; 128.60; 128.00; 127.42; 126.13; 122.65; 118.11; 90.33; 18.02; HRMS[ESI]: calculated for C₁₈H₁₆NO₂, [M+H]⁺: 278.1176, found: 278.1178.





3c



¹H NMR (400 MHz, CDCl₃): 8.13 (d, J = 7.6 Hz, 2H); 8.08 (d, J = 8.4 Hz, 1H); 8.00 (d, J = 9.2 Hz, 1H); 7.60-7.52 (m, 2H); 7.47-7.44 (m, 2H); 7.39-7.37 (m, 1H); 7.08 (s, 1H); 5.63 (s, 2H); 3.93 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.33; 157.97; 153.70; 143.69; 135.81; 133.21; 130.56; 129.93; 129.86; 128.65; 128.46; 122.68; 119.96; 105.08; 67.91; 55.58; HRMS[ESI]: calculated for C₁₈H₁₆NO₃, [M+H]⁺: 294.1125, found: 294.1127.





3d



¹H NMR (400 MHz, CDCl₃): 9.05 (s, 1H); 8.14-8.09 (m, 4H); 7.81-7.79 (m, 2H); 7.62-7.58 (m, 1H); 7.49-7.45 (m, 2H); 5.70 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.17; 151.03; 144.21; 142.21; 141.85; 133.48; 130.48; 130.19; 129.90; 129.44; 129.37; 129.31; 128.56; 66.04; HRMS[ESI]: calculated for $C_{16}H_{13}N_2O_2$, $[M+H]^+$: 265.0972, found: 265.0975.





3e



¹H NMR (400 MHz, CDCl₃): 8.15-8.10 (m, 3H); 7.99-7.95 (m, 2H); 7.81-7.78 (m, 1H); 7.62-7.58 (m, 2H); 7.47 (t, J = 7.6 Hz, 2H); 5.63 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.24; 156.92; 146.20; 136.06; 133.49; 133.36; 130.91; 130.20; 129.86; 129.68; 128.64; 128.52; 120.60; 120.21; 67.64; HRMS[ESI]: calculated for C₁₇H₁₂BrNO₂Na, [M+Na]⁺: 363.9944, found: 363.9948.





¹H NMR (400 MHz, CDCl₃): 8.15-8.10 (m, 3H); 8.00 (d, J = 8.4 Hz, 1H); 7.59-7.53 (m, 4H); 7.48-7.44 (m, 2H); 5.65 (s, 2H); 2.54 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.31; 155.37; 136.67; 136.45; 133.24; 132.23; 129.87; 128.78; 128.57; 128.47; 127.65; 126.60; 126.49; 119.50; 67.92; 21.61; HRMS[ESI]: calculated for C₁₈H₁₆NO₂, [M+H]⁺: 278.1176, found: 278.1178.

3g

¹H NMR (400 MHz, CDCl₃): 8.23 (d, J = 8.0 Hz, 1H); 8.16-8.11 (m, 3H); 7.82-7.77 (m, 1H); 7.67-7.59 (m, 3H); 7.51-7.47 (m, 2H); 5.63 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.17; 156.41; 148.45; 143.57; 133.41; 130.79; 129.90; 129.60; 129.55; 128.55; 127.71; 125.79; 124.10; 119.47; 67.32; HRMS[ESI]: calculated for C₁₇H₁₂ClNO₂Na, [M+Na]⁺: 320.0448, found: 320.0451.

¹H NMR (400 MHz, CDCl₃): 8.15-8.07 (m, 4H); 7.60-7.57 (m, 2H); 7.53-7.42 (m, 4H); 5.64 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.27; 155.78; 144.66; 136.47; 133.35; 133.31; 131.71; 129.89; 129.86; 128.54; 128.50; 120.27; 110.76; 110.58; 67.67; HRMS[ESI]: calculated for $C_{17}H_{13}FNO_2$, $[M+H]^+$: 282.0925, found: 282.0926.

¹H NMR (400 MHz, CDCl₃): 8.22-8.15 (m, 3H); 7.84 (d, J = 7.2 Hz, 1H); 7.75 (d, J = 8.0 Hz, 1H); 7.64-7.58 (m, 2H); 7.50-7.44 (m, 3H); 5.75 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.26; 157.43; 143.89; 137.46; 133.43; 133.31; 130.00; 129.87; 129.82; 128.86; 128.52; 126.79; 126.56; 119.96; 67.74; HRMS[ESI]: calculated for C₁₇H₁₃ClNO₂, [M+H]⁺: 298.0629, found: 298.0634.

3j

¹H NMR (400 MHz, CDCl₃): 8.18-8.09 (m, 4H); 7.76 (d, J = 8.8 Hz, 1H); 7.62-7.55 (m, 2H); 7.51-7.45 (m, 3H); 5.64 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.24; 157.58; 147.94; 136.89; 135.77; 133.36; 129.87; 129.71; 128.85; 128.53; 128.22; 127.80; 125.90; 119.47; 67.56; HRMS[ESI]: calculated for C₁₇H₁₃ClNO₂, [M+H]⁺: 298.0629, found: 298.0626.

¹H NMR (400 MHz, CDCl₃): 8.72 (s, 1H); 8.23 (d, J = 8.4 Hz, 1H); 8.14 (t, J = 8.8 Hz, 2H); 7.97 (d, J = 8.0 Hz, 1H); 7.92-7.84 (m, 3H); 7.75 (t, J = 7.2 Hz, 1H); 7.65-7.54 (m, 4H); 5.74 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 165.43; 155.38; 146.61; 136.11; 134.64; 131.46; 130.44; 128.88; 128.39; 128.14; 127.39; 127.25; 126.77; 126.63; 126.57; 125.99; 125.71; 124.31; 121.36; 118.48; 66.96; HRMS[ESI]: calculated for C₂₁H₁₆NO₂, [M+H]⁺: 314.1176, found: 314.1174.

¹H NMR (400 MHz, CDCl₃): 8.30-8.29 (m, 2H); 8.11 (s, 1H); 8.03 (d, J = 7.6 Hz, 1H); 7.88 (d, J = 7.6 Hz, 1H); 7.82-7.78 (m, 1H); 7.62-7.56 (m, 3H); 7.42 (t, J = 7.6 Hz, 1H); 5.74 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 165.12; 155.91; 147.69; 137.17; 134.66; 133.81; 133.31; 131.58; 129.97; 129.91; 129.83; 129.23; 128.01; 127.68; 126.83; 119.46; 68.26; HRMS[ESI]: calculated for C₁₇H₁₃ClNO₂, [M+H]⁺: 298.0629, found: 298.0629.

 $3\mathbf{m}$

¹H NMR (300 MHz, CDCl₃): 8.22-8.09 (m, 4H); 7.84 (d, J = 8.1 Hz, 1H); 7.77-7.72 (m, 1H); 7.59-7.55 (m, 2H); 7.13 (t, J = 8.4 Hz, 2H); 5.65 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 167.25; 165.33; 164.72; 156.08; 137.51; 137.43; 132.51; 132.42; 127.68; 127.62; 126.94; 119.48; 115.80; 115.58; 67.77; HRMS[ESI]: calculated for C₁₇H₁₃FNO₂, [M+H]⁺: 282.0925, found: 282.0932.

¹H NMR (400 MHz, CDCl₃): 8.21 (d, J = 8.8 Hz, 1H); 8.13 (d, J = 8.4 Hz, 1H); 8.03 (d, J = 8.0 Hz, 2H); 7.84 (d, J = 8.0 Hz, 1H); 7.75 (t, J = 7.2 Hz, 1H); 7.59-7.54 (m, 2H); 7.28-7.26 (m, 2H); 5.67 (s, 2H); 2.42 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.33; 156.53; 147.39; 144.04; 137.28; 130.02; 129.92; 129.21; 128.99; 127.66; 127.60; 127.07; 126.79; 119.42; 67.53; 21.72; HRMS[ESI]: calculated for C₁₈H₁₆NO₂, [M+H]⁺: 278.1176, found: 278.1179.

¹H NMR (400 MHz, CDCl₃): 8.20 (d, J = 8.4 Hz, 1H); 8.11 (d, J = 8.4 Hz, 1H); 7.95-7.94 (m, 2H); 7.83 (d, J = 8.0 Hz, 1H); 7.74 (t, J = 7.2 Hz, 1H); 7.59-7.54 (m, 2H); 7.41-7.33 (m, 2H); 5.66 (s, 2H); 2.41 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.46; 156.45; 147.57; 138.30; 137.14; 134.04; 130.39; 129.92; 129.75; 129.12; 128.38; 127.65; 127.59; 127.01; 126.73; 119.44; 67.77; 21.29; HRMS[ESI]: calculated for C₁₈H₁₆NO₂, [M+H]⁺: 278.1176, found: 278.1175.

¹H NMR (400 MHz, CDCl₃): 8.24 (d, J = 7.6 Hz, 1H); 8.15 (d, J = 7.2 Hz, 1H); 7.97 (d, J = 7.2 Hz, 1H); 7.85 (d, J = 7.2 Hz, 1H); 7.76-7.74 (m, 1H); 7.64-7.62 (m, 1H); 7.59-7.56 (m, 1H); 7.48-7.45 (m, 2H); 7.36-7.34 (m, 1H); 5.70 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 165.28; 155.80; 137.52; 134.03; 132.90; 131.80; 131.21; 130.18; 129.65; 128.87; 127.69; 127.64; 126.95; 126.70; 119.67; 119.58; 68.04; HRMS[ESI]: calculated for C₁₇H₁₃ClNO₂, [M+H]⁺: 298.0629, found: 298.0635.

3q

¹H NMR (400 MHz, CDCl₃): 8.23 (d, J = 8.4 Hz, 1H); 8.13 (d, J = 8.4 Hz, 1H); 8.07 (d, J = 8.4 Hz, 2H); 7.85 (d, J = 8.0 Hz, 1H); 7.76 (t, J = 7.2 Hz, 1H); 7.60-7.56 (m, 2H); 7.44 (d, J = 8.0 Hz, 2H); 5.67 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 165.45; 155.96; 139.80; 131.27; 130.13; 128.99; 128.86; 128.24; 127.67; 127.62; 127.43; 126.93; 119.48; 112.05; 67.90; HRMS[ESI]: calculated for C₁₇H₁₃ClNO₂, [M+H]⁺: 298.0629, found: 298.0635.

3r

¹H NMR (400 MHz, CDCl₃): 8.22 (d, J = 8.4 Hz, 1H); 8.10 (d, J = 8.4 Hz, 1H); 7.94 (d, J = 8.0 Hz, 1H); 7.85-7.82 (m, 2H); 7.75-7.63 (m, 3H); 7.58-7.54 (m, 2H); 5.66 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 165.14; 155.07; 148.17; 147.40; 137.41; 133.08; 131.97; 130.14; 130.03; 129.04; 127.70; 127.38; 127.05; 126.94; 124.03; 119.69; 69.08; HRMS[ESI]: calculated for C₁₇H₁₃N₂O₄, [M+H]⁺: 309.0870, found: 309.0875.

¹H NMR (400 MHz, CDCl₃): 8.29-8.27 (m, 2H); 8.21 (d, J = 7.6 Hz, 1H); 8.07 (d, J = 7.6 Hz, 1H); 7.87 (d, J = 8.0 Hz, 1H); 7.79 (t, J = 7.2 Hz, 1H); 7.72 (d, J = 8.0 Hz, 1H); 7.62-7.58 (m, 2H); 7.35 (t, J = 7.6 Hz, 1H); 5.72 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 164.98; 155.84; 147.53; 137.30; 136.22; 133.04; 132.82; 131.74; 130.07; 129.11; 128.46; 127.68; 127.62; 126.89; 122.57; 119.48; 68.15; HRMS[ESI]: calculated for C₁₇H₁₃BrNO₂, [M+H]⁺: 342.0124, found: 342.0120.

¹H NMR (400 MHz, CDCl₃): 8.21 (d, J = 8.4 Hz, 1H); 8.10 (d, J = 8.8 Hz, 1H); 7.90 (dd, J = 1.2 Hz, J = 4.0 Hz, 1H); 7.83 (d, J = 8.0 Hz, 1H); 7.74 (td, J = 1.6 Hz, J = 6.8 Hz, 1H); 7.61-7.54 (m, 3H); 7.13 (dd, J = 3.6 Hz, J = 5.0 Hz, 1H); 5.64 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 161.89; 156.16; 147,52; 137.20; 134.05; 133.21; 132.92; 129.96; 129.09; 127.93; 127.67; 127.60; 126.77; 119.33; 67.81; HRMS[ESI]: calculated for C₁₅H₁₂NO₂S, [M+H]⁺: 270.0583, found: 270.0587.

¹H NMR (400 MHz, CDCl₃): 8.11-8.09 (m, 2H); 7.59-7.55 (m, 1H); 7.48-7.36 (m, 7H); 5.38 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.39; 136.01; 133.00; 130.08; 129.67; 128.56; 128.34; 128.21; 128.13; 66.65;

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¹H NMR (400 MHz, CDCl₃): 8.13 (d, J = 8.4 Hz, 2H); 7.60 (t, J = 7.2 Hz, 1H); 7.48 (t, J = 7.6 Hz, 2H); 7.34-7.29 (m, 3H); 7.20 (d, J = 7.2 Hz, 1H); 5.38 (s, 2H); 2.42 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.41; 138.24; 135.94; 132.95; 130.16; 129.67; 128.96; 128.89; 128.47; 128.31; 125.23; 66.71; 21.35; HRMS (ESI): calculated for C₁₅H₁₄O₂Na, [M+Na]⁺: 249.0886, found 249.0888.

¹H NMR (400 MHz, CDCl₃): 8.10 (d, J = 7.2 Hz, 2H); 7.57 (t, J = 7.2 Hz, 1H); 7.44 (t, J = 8.0 Hz, 2H); 7.37 (d, J = 8.0 Hz, 2H); 7.22 (d, J = 8.0 Hz, 2H); 5.35 (s, 2H); 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.42; 138.03; 133.00; 132.91; 130.18; 129.64; 129.22; 128.29; 128.29; 66.61; 21.17; HRMS (ESI): calculated for C₁₅H₁₄O₂Na, [M+Na]⁺: 249.0886, found 249.0888.

¹H NMR (400 MHz, CDCl₃): 8.12 (d, J = 7.2 Hz, 2H); 7.60 (t, J = 7.6 Hz, 1H); 7.50-7.46 (m, 3H); 7.32-7.27 (m, 3H); 5.43 (s, 2H); 2.46 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.47; 137.12; 134.02; 133.05; 130.45; 130.18; 129.72; 129.30; 128.60; 128.42; 126.09; 65.26; 19.05;

¹H NMR (400 MHz, CDCl₃): 8.07 (d, J = 7.2 Hz, 2H); 7.57 (t, J = 7.2 Hz, 1H); 7.46-7.42 (m, 4H); 7.08 (t, J = 8.4 Hz, 2H); 5.33 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.40; 163.92; 133.14; 130.27; 130.19; 129.71; 128.43; 115.66; 115.45; 66.01; HRMS (ESI): calculated for C₁₄H₁₁FO₂Na, [M+Na]⁺: 253.0635, found 253.0631.

¹H NMR (400 MHz, CDCl₃): 8.09 (d, J = 8.0 Hz, 2H); 7.58 (t, J = 7.6 Hz, 1H); 7.48-7.44 (m, 3H); 7.33 (s, 3H); 5.34 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.27; 138.08; 134.51; 133.23; 129.92; 129.86; 129.75; 128.47; 128.42; 128.15; 126.16; 65.78; HRMS (ESI): calculated for C₁₄H₁₁ClO₂Na, [M+Na]⁺: 269.0340, found 269.0339.

¹H NMR (400 MHz, CDCl₃): 8.07 (d, J = 8.0 Hz, 2H); 7.55 (t, J = 7.2 Hz, 1H); 7.42 (q, J = 7.6 Hz, 4H); 6.92 (d, J = 8.4 Hz, 2H); 5.31 (s, 2H); 3.82 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 166.53; 159.68; 132.96; 130.30; 130.09; 129.69; 128.35; 128.21; 114.00; 66.56; 55.31; HRMS (ESI): calculated for C₁₅H₁₄O₃Na, [M+Na]⁺: 265.0835, found 265.0829.

¹H NMR (400 MHz, CDCl₃): 8.21 (d, J = 7.2 Hz, 2H); 7.60 (t, J = 7.2 Hz, 1H); 7.51-7.47 (m, 6H); 7.40 (t, J = 7.2 Hz, 4H); 7.33 (t, J = 7.2 Hz, 2H); 7.19 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): 165.49; 140.23; 133.09; 130.16; 129.73; 128.51; 128.39; 127.91; 127.08; 76.68;

¹H NMR (400 MHz, CDCl₃): 8.13 (d, J = 8.0 Hz, 2H); 7.93-7.86 (m, 4H); 7.60-7.56 (m, 2H); 7.53-7.49 (m, 2H); 7.46 (t, J = 7.6 Hz, 2H); 5.55 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 166.52; 133.51; 133.27; 133.19; 133.11; 130.18; 129.78; 128.45; 128.45; 128.06; 127.78; 127.38; 126.37; 126.33; 125.94; 66.92;

¹H NMR (400 MHz, CDCl₃): 8.12 (d, J = 8.0 Hz, 2H); 7.57 (t, J = 7.2 Hz, 1H); 7.49-7.44 (m, 4H); 7.40 (t, J = 7.2 Hz, 2H); 7.32 (t, J = 6.8 Hz, 1H); 6.17 (q, J = 6.8 Hz, 1H); 1.71 (d, J = 6.4 Hz, 3H); 1³C NMR (100 MHz, CDCl₃): 165.74; 141.73; 132.86; 130.46; 129.59; 128.50; 128.28; 127.83; 125.99; 72.85; 22.37;

¹H NMR (400 MHz, CDCl₃): 8.14 (d, J = 7.6 Hz, 2H); 7.93-7.85 (m, 4H); 7.62-7.56 (m, 2H); 7.51-7.45 (m, 4H); 6.34 (q, J = 6.4 Hz, 1H); 1.79 (d, J = 6.8 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): 165.90; 139.15; 133.25; 133.10; 132.99; 130.57; 129.72; 128.49; 128.41; 128.11; 127.72; 126.28; 126.12; 125.05; 124.12; 73.11; 22.39; HRMS (ESI): calculated for C₁₉H₁₆O₂Na, [M+Na]⁺: 299.1043, found 299.1043.

¹H NMR (400 MHz, CDCl₃): 8.10-8.05 (m, 4H); 7.58 (t, J = 7.2 Hz, 1H); 7.51 (d, J = 8.0 Hz, 2H); 7.46 (t, J = 7.6 Hz, 2H); 5.42 (s, 2H); 3.92 (s, 3H);¹³C NMR (100 MHz, CDCl₃): 166.71; 166.24; 141.08; 133.21; 129.88; 129.88; 129.78; 129.70; 128.44; 127.61; 65.88; 52.16; HRMS (ESI): calculated for C₁₆H₁₄O₄Na, [M+Na]⁺: 293.0784, found 293.0785.

