



Advanced
**Synthesis &
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Supporting Information

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Efficient carbonylation of aryl and heteroaryl bromides using a Palladium/diadamantylbutylphosphine catalyst

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Supporting Information

Butyl 4-methoxybenzoate

R_f (SiO₂, *n*-heptane/EtOAc = 10/0.5): 0.18. Yield: 80 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 7.99 (d, *J* = 8.9 Hz, 2H, 2CH), 6.91 (d, *J* = 8.9 Hz, 2H, 2CH), 4.29 (t, *J* = 6.6 Hz, 2H, OCH₂), 3.85 (s, 3H, OCH₃), 1.73 (quin, *J* ≈ 7.1 Hz, 2H, OCH₂CH₂), 1.47 (sext, *J* ≈ 7.4 Hz, 2H, CH₂CH₃), 0.97 (t, *J* = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 166.4 and 163.2 (C=O, OC=), 131.5 and 113.5 (4CH), 163.2 (C), 64.5, 30.8 and 19.2 (3CH₂), 55.3 and 13.7 (2CH₃). MS (EI, 70 eV): *m/z* (%) = 208 (15) [M]⁺, 152 (100), 135 (99) [M-OBu]⁺, 77 (10), no other peaks > 10%. IR (KBr): 1/λ = 2960 (m), 2874 (w), 1712 (s), 1607 (s), 1582 (w), 1512 (s), 1464 (m), 1420 (w), 1384 (w), 1316 (m), 1277 (s), 1257 (s), 1168 (s), 1102 (s), 1031 (m), 847 (m), 771 (m), 697 (w), 613 (w) cm⁻¹. HR-MS (EI): calc. for C₁₂H₁₆O₃: 208.1094; found: 208.1088 [M]⁺.

Butyl 2-cyanobenzoate

R_f (SiO₂, *n*-heptane/EtOAc = 10/1): 0.16. Yield: 78 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 8.14 (dd, J = 6.9, 2.2 Hz, 1H, CH), 7.80 (dd, J = 6.7, 2.5 Hz, 1H, CH), 7.66 (m, 2H, CH), 4.41 (t, J = 6.7 Hz, 2H, OCH₂), 1.80 (quin, J \approx 7.1 Hz, 2H, OCH₂CH₂), 1.49 (sext, J \approx 7.5 Hz, 2H, CH₂CH₃), 0.97 (t, J = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 164.1 (C=O), 134.8, 132.5, 132.4 and 131.1 (4C), 132.7, 117.5 and 112.8 (3CH), 66.1, 30.4 and 19.2 (3CH₂), 13.7 (CH₃). MS (EI, 70 eV): m/z (%) = 203 (1) [M]⁺, 148 (66), 130 (100) [M-OBu]⁺, 102 (27), 56 (9), no other peaks > 10%. IR (KBr): $1/\lambda$ = 2962 (s), 2874 (s), 2229 (m, CN), 1725 (s), 1595 (w), 1577 (w), 1488 (w), 1386 (w), 1279 (s), 1140 (m), 1082 (s), 940 (w), 761 (s), 694 (m), 661 (w) cm⁻¹. HR-MS (EI): calc. for C₁₂H₁₃NO₂: 203.0941; found: 203.0935 [M]⁺.

Butyl 4-cyanobenzoate

R_f (SiO₂, *n*-heptane/EtOAc = 10/0.25): 0.14. Yield: 82 %. White solid, m.p.: 48°C. ¹H NMR (400 MHz, CDCl₃): δ = 8.13 (d, J = 8.6 Hz, 2H, 2CH), 7.74 (d, J = 8.6 Hz, 2H, 2CH), 4.40 (t, J = 6.6 Hz, 2H, OCH₂), 1.76 (quin, J \approx 7.1 Hz, 2H, OCH₂CH₂), 1.47 (sext, J \approx 7.4 Hz, 2H, CH₂CH₃), 0.98 (t, J = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 165.0 (C=O), 132.2 and 130.0 (4CH), 134.3, 118.0 and 116.2 (3C), 65.6, 30.6 and 19.2 (3CH₂), 13.7 (CH₃). MS (EI, 70 eV): m/z (%) = 203 (2) [M]⁺, 148 (42), 130 (100) [M-OBu]⁺, 102 (53), 75 (12), 56 (32), 41 (10), no other peaks > 10%. IR (KBr): $1/\lambda$ = 3414 (m), 3102 (w), 3071 (m), 2957 (s), 2938 (s), 2874 (s), 2233 (s, CN), 1713 (s), 1610 (w), 1569 (w), 1468 (m), 1411 (m), 1355 (m), 1317 (s), 1284 (s), 1263 (s), 1184 (m), 1119 (s), 1021 (w), 964 (m), 906 (w), 868 (m), 767 (s), 739 (w), 692 (m), 643 (w), 546 (m) cm⁻¹. HR-MS (EI): calc. for C₁₂H₁₃NO₂: 203.0941; found: 203.0939 [M]⁺.

Butyl 4-(dimethylamino)benzoate

R_f (SiO₂, *n*-heptane/EtOAc = 10/0.25): 0.15. Yield: 80 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 7.91 (d, *J* = 9.2 Hz, 2H, CH), 6.64 (d, *J* = 9.2 Hz, 2H, CH), 4.26 (t, *J* = 6.6 Hz, 2H, OCH₂), 3.03 (s, 6H, N(CH₃)₂), 1.73 (quin, *J* ≈ 7.1 Hz, 2H, OCH₂CH₂), 1.47 (sext, *J* ≈ 7.4 Hz, 2H, CH₂CH₃), 0.97 (t, *J* = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 167.1 (C=O), 153.2, 117.3 (2C), 131.2 and 110.7 (2CH), 64.0, 31.0 and 19.3 (3CH₂), 40.1 (NCH₃)₂, 13.8 (CH₃). MS (EI, 70 eV): *m/z* (%) = 221 (91) [M]⁺, 165 (100), 164 (71) [M-Bu]⁺, 148 (94) [M-OBu]⁺, no other peaks > 10%. IR (KBr): 1/λ = 2959 (s), 1701 (s), 1609 (s), 1526 (m), 1447 (m), 1368 (s), 1279 (s), 1184 (s), 1106 (s), 1065 (w), 947 (w), 830 (w), 770 (m), 699 (w) cm⁻¹. HR-MS (EI): calc. for C₁₃H₁₉NO₂: 221.1410; found: 221.1405 [M]⁺.

Butyl thiophene-2-carboxylate

R_f (SiO₂, *n*-heptane/EtOAc = 10/0.25): 0.15. Yield: 52 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 7.79 (dd, *J* = 3.7, 1.3 Hz, 1H, CH), 7.53 (dd, *J* = 5.0, 1.3 Hz, 1H, CH), 7.01 (dd, *J* = 3.7, 5.0 Hz, 1H, CH), 4.30 (t, *J* = 6.6 Hz, 2H, OCH₂), 1.73 (quin, *J* ≈ 7.1 Hz, 2H, OCH₂CH₂), 1.46 (sext, *J* ≈ 7.4 Hz, 2H, CH₂CH₃), 0.97 (t, *J* = 7.4 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 162.3 (C=O), 134.1 (C), 133.18, 132.1 and 127.7 (3CH), 65.0, 30.7 and 19.2 (3CH₂), 13.7 (CH₃). MS (EI, 70 eV): *m/z* (%) = 284 (9) [M]⁺, 229 (11), 211 (31) [M-OBu]⁺, 184 (12), 173 (29), 172 (25), 155 (50), 129 (20), 128 (50), 111 (100), 83 (11), 56 (15), no other peaks > 10%. IR (KBr): 1/λ = 3106 (w), 2960 (s), 1709 (s), 1526 (s), 1465 (m), 1420 (s), 1383 (m), 1359 (s), 1260 (s), 1225 (s), 1094 (s), 1038 (m), 941 (w), 861 (m), 752 (s), 719 (s) cm⁻¹. HR-MS (EI): calc. for C₉H₁₂SO₂: 184.0553; found: 184.0550 [M]⁺.

Butyl thiophene-3-carboxylate

R_f (SiO₂, *n*-heptane): 0.08. Yield: 77 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 8.09 (dd, J = 3.1, 1.2 Hz, 1H, CH), 7.52 (dd, J = 5.1, 1.2 Hz, 1H, CH), 7.30 (dd, J = 3.1, 5.1 Hz, 1H, CH), 4.28 (t, J = 6.7 Hz, 2H, OCH₂), 1.72 (quin, J \approx 7.1 Hz, 2H, OCH₂CH₂), 1.46 (sext, J \approx 7.4 Hz, 2H, CH₂CH₃), 0.97 (t, J = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 162.9 (C=O), 134.0 (C), 132.4, 127.9 and 125.9 (3CH), 64.5, 30.8 and 19.2 (3CH₂), 13.7 (CH₃). MS (EI, 70 eV): m/z (%) = 184 (17) [M]⁺, 129 (40), 128 (83), 111 (100) [M-OBu]⁺, 85 (14), 83 (38), 56 (91), no other peaks > 10%. IR (KBr): $1/\lambda$ = 3113 (s), 2960 (s), 2874 (m), 1717 (s), 1524 (m), 1465 (w), 1412 (m), 1379 (w), 1261 (s), 1204 (s), 1189 (s), 1104 (s), 1018 (w), 996 (w), 947 (w), 872 (w), 823 (w), 749 (s) cm⁻¹. HR-MS (EI): calc. for C₉H₁₂SO₂: 184.0553; found: 184.0550 [M]⁺.

Butyl benzo[b]thiophene-3-carboxylate

R_f (SiO₂, *n*-heptane): 0.09. Yield: 83 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 8.60 (d, J = 8.4 Hz, 1H, CH), 8.38 (s, 1H, SCH), 7.87 (d, J = 8.1 Hz, 1H, CH), 7.49 (ddd, J = 8.4, 7.2 and 1.3 Hz, 1H, CH), 7.41 (ddd, J = 8.1, 7.2 and 1.3 Hz, 1H, CH), 4.38 (t, J = 6.6 Hz, 2H, OCH₂), 1.80 (quin, J \approx 7.1 Hz, 2H, OCH₂CH₂), 1.52 (sext, J \approx 7.4 Hz, 2H, CH₂CH₃), 1.00 (t, J = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 162.9 (C=O), 140.0, 136.7 and 127.4 (3C), 136.4, 125.3, 124.9 and 124.7 (4CH), 64.5, 30.8 and 19.3 (3CH₂), 13.8 (CH₃). MS (EI, 70 eV): m/z (%) = 234 (61) [M]⁺, 178 (100), 161 (92) [M-OBu]⁺, 134 (24), 89 (37), no other peaks > 10%. IR (KBr): $1/\lambda$ = 3109 (w), 2959 (s), 2872 (w), 1712 (s), 1505 (m), 1463 (m), 1423 (m), 1392 (w), 1366 (w), 1261 (m), 1218 (s), 1148 (w), 1129 (w), 1068 (m), 1019 (w), 865 (w), 770 (s), 746 (m), 723 (m) cm⁻¹. HR-MS (EI): calc. for C₁₃H₁₄SO₂: 234.0709; found: 234.0708 [M]⁺.

Butyl 6-methoxy-2-naphthoate

R_f (SiO₂, *n*-heptane/EtOAc = 10/0.25): 0.15. Yield: 95 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 8.52 (d, J = 1.7 Hz, 1H, CH), 8.03 (dd, J = 8.6, 1.7 Hz, 1H, CH), 7.84 (d, J = 8.8 Hz, 1H, CH), 7.75 (d, J = 8.7 Hz, 1H, CH), 7.19 (dd, J = 9.0, 2.6 Hz, 1H, CH), 7.14 (d, J = 2.6 Hz, 1H, CH), 4.38 (t, J = 6.6 Hz, 2H, OCH₂), 3.93 (s, 1H, OMe), 1.80 (quin, J \approx 7.0 Hz, 2H, OCH₂CH₂), 1.52 (sext, J \approx 7.5 Hz, 2H, CH₂CH₃), 1.00 (t, J = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 166.9 (C=O), 159.4, 137.1, 127.9 and 125.5 (4C), 130.8, 130.7, 126.7, 125.9, 119.5 and 105.6 (6CH), 64.8, 30.8 and 19.3 (3CH₂), 55.3 (OCH₃), 13.8 (CH₃). MS (EI, 70 eV): m/z (%) = 258 (36) [M]⁺, 202 (100), 185 (49) [M-OBu]⁺, 178 (20), 161 (15), 159 (12), 157 (23), 142 (13), 114 (16), no other peaks > 10%. IR (KBr): $1/\lambda$ = 2959 (s), 2873 (m), 1713 (s), 1629 (s), 1606 (m), 1506 (m), 1482 (s), 1415 (w), 1389 (s), 1339 (m), 1279 (s), 1204 (s), 1125 (w), 1096 (s), 1031 (m), 967 (w), 913 (w), 857 (m), 822 (m), 767 (m), 751 (m) cm⁻¹. HR-MS (EI): calc. for C₁₆H₁₈O₃: 258.1250; found: 258.1248 [M]⁺.

Butyl benzo[d][1,3]dioxole-5-carboxylate

R_f (SiO₂, *n*-heptane/EtOAc = 10/0.25): 0.14. Yield: 78 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 7.64 (dd, J = 8.2, 1.7 Hz, 1H, CH), 7.46 (d, J = 1.7 Hz, 1H, CH), 6.83 (d, J = 8.2 Hz, 1H, CH), 6.03 (s, 2H, OCH₂O), 4.28 (t, J = 6.6 Hz, 2H, OCH₂), 1.73 (quin, J \approx 7.1 Hz, 2H, OCH₂CH₂), 1.46 (sext, J \approx 7.5 Hz, 2H, CH₂CH₃), 0.97 (t, J = 7.4 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 166.0 (C=O), 151.4, 147.6 and 124.5 (3C), 125.2, 109.4 and 107.9 (3CH), 101.7 (OCH₂O), 64.7, 30.8 and 19.2 (3CH₂), 13.7 (CH₃). MS (EI, 70 eV): m/z (%) = 222 (25) [M]⁺, 166 (100), 149 (70) [M-OBu]⁺, 121 (12), no other peaks > 10%. IR (KBr): $1/\lambda$ = 2960 (s), 1713 (s), 1626 (m), 1608 (m), 1490 (s), 1443 (s), 1385 (m), 1364 (m), 1280 (s), 1258 (s), 1159 (s), 1105 (s), 1076 (s), 1039 (s), 937 (m), 881 (m), 828 (w), 808 (m), 762 (s), 721 (w), 680 (w) cm⁻¹. HR-MS (EI): calc. for C₁₂H₁₄O₄: 222.0887; found: 222.0883 [M]⁺.

Butyl 4-chlorobenzoate

R_f (SiO₂, *n*-heptane): 0.09. Yield: 78 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 7.97 (d, J = 8.9 Hz, 2H, 2CH), 7.40 (d, J = 8.9 Hz, 2H, 2CH), 4.32 (t, J = 6.7 Hz, 2H, OCH₂), 1.75 (quin, J \approx 7.1 Hz, 2H, OCH₂CH₂), 1.47 (sext, J \approx 7.4 Hz, 2H, CH₂CH₃), 0.98 (t, J = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 165.8 (C=O), 139.2 and 120.0 (2C), 130.9 and 128.7 (4CH), 65.1, 30.7 and 19.2 (3CH₂), 13.7 (CH₃). MS (EI, 70 eV): m/z (%) = 212 (1) [M]⁺, 159 (14), 158 (19), 157 (43), 156 (50), 141 (35), 139 (100) [M-OBu]⁺, 113 (15), 111 (39), 75 (22), 56 (33), no other peaks > 10%. IR (KBr): $1/\lambda$ = 2961 (s), 2874 (s), 1720 (s), 1596 (s), 1488 (s), 1466 (m), 1402 (s), 1274 (s), 1172 (s), 1104 (s), 1016 (s), 964 (w), 850 (s), 760 (s), 685 (m), 629 (w) cm⁻¹. HR-MS (EI): calc. for C₁₁H₁₃ClO₂: 212.0599; found: 212.0601 [M]⁺.

Butyl 3,4,5-trifluorobenzoate

R_f (SiO₂, *n*-heptane/EtOAc = 10/1): 0.59. Yield: 73 %. Colorless oil. ¹H NMR (400 MHz, CDCl₃): δ = 7.67 (m, 2H, 2CH), 4.33 (t, J = 6.7 Hz, 2H, OCH₂), 1.75 (quin, J \approx 7.1 Hz, 2H, OCH₂CH₂), 1.46 (sext, J \approx 7.4 Hz, 2H, CH₂CH₃), 0.98 (t, J = 7.3 Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ = 163.8 (C=O), 151.0 (J = 255 Hz, CF), 143.0 (J = 259 Hz, CF), 126.4 (C), 114.1 (2CH), 65.8, 30.6 and 19.2 (3CH₂), 13.7 (CH₃). MS (EI, 70 eV): m/z (%) = 232 (0.3) [M]⁺, 177 (12), 159 (100) [M-OBu]⁺, 131 (43), 81 (21), 56 (84), 41 (17), no other peaks > 10%. IR (KBr): $1/\lambda$ = 3086 (w), 2964 (s), 1732 (s), 1625 (s), 1529 (s), 1441 (s), 1392 (s), 1353 (s), 1252 (s), 1223 (s), 1086 (m), 1049 (s), 968 (w), 889 (m), 767 (s), 738 (m), 713 (w) cm⁻¹. HR-MS (EI): calc. for C₁₁H₁₁F₃O₂: 232.0706; found: 232.0706 [M]⁺.

Butyl quinoxaline-6-carboxylate

R_f (SiO₂, *n*-heptane/EtOAc = 4/1): 0.35. Yield: 51 %. Yellow solid, m.p.: 39°C. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 9.05 (s, 2H, NCH=CHN), 8.58 (d, J = 1.8 Hz, 1H, COCHCN), 8.27 (dd, J =

8.9, 1.8 Hz, 1H, COCHCH), 8.18 (d, $J = 8.9$ Hz, 1H, COCHCH), 4.34 (t, $J = 6.6$ Hz, 2H, OCH₂), 1.73 (quin, $J \approx 7.1$ Hz, 2H, OCH₂CH₂), 1.44 (sext, $J \approx 7.4$ Hz, 2H, CH₂CH₃), 0.98 (t, $J = 7.3$ Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, DMSO-*d*₆): $\delta = 164.9$ (C=O), 147.7, 147.0, 131.0, 129.9 and 128.9 (5CH), 144.1, 141.4 and 130.9 (3C), 65.0, 30.1 and 18.7 (3CH₂), 13.6 (CH₃). MS (EI, 70 eV): m/z (%) = 230 (125) [M]⁺, 174 (90), 157 (100) [M-OBu]⁺, 129 (45), 102 (26), 75 (13), no other peaks > 10%. IR (KBr): $1/\lambda = 2958$ (m), 2875 (w), 1723 (s), 1487 (m), 1448 (w), 1423 (m), 1361 (m), 1308 (s), 1282 (s), 1242 (m), 1207 (w), 1176 (s), 1132 (m), 1089 (m), 1020 (m), 965 (w), 956 (w), 908 (m), 872 (m), 846 (w), 812 (w), 754 (s) cm⁻¹. HR-MS (EI): calc. for C₁₃H₁₄N₂O₂: 230.1055; found: 230.1050 [M]⁺.

Butyl 2,5-bis(trifluoromethyl)benzoate

R_f (SiO₂, *n*-heptane/EtOAc = 10/0.5): 0.43. Yield: 76 %. Yellow oil. ¹H NMR (400 MHz, CDCl₃): $\delta = 8.04$ (s, 1H, CH), 7.88 (m, 2H, 2CH), 4.37 (t, $J = 6.7$ Hz, 2H, OCH₂), 1.76 (quin, $J \approx 7.2$ Hz, 2H, OCH₂CH₂), 1.45 (sext, $J \approx 7.5$ Hz, 2H, CH₂CH₃), 0.97 (t, $J = 7.3$ Hz, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): $\delta = 165.6$ (C=O), 134.0 (q, $J = 34$ Hz, CCF₃), 131.9 (q, $J = 35$ Hz, CCF₃), 127.9 (q, $J = 3.4$ Hz, CH), 127.6 (q, $J = 5.5$ Hz, CH), 127.4 (q, $J = 3.9$ Hz, CH), 122.5 (q, $J = 269$ Hz, CF₃), 122.7 (q, $J = 269$ Hz, CF₃), 66.6, 30.3 and 19.0 (3CH₂), 13.6 (CH₃). MS (EI, 70 eV): m/z (%) = 295 (4) [M-F]⁺, 241 (55) [M-OBu]⁺, 213 (16), 163 (27), 56 (100), 41 (25), no other peaks > 10%. IR (KBr): $1/\lambda = 2966$ (s), 2879 (m), 1742 (s), 1626 (w), 1509 (w), 1468 (m), 1418 (m), 1387 (m), 1340 (s), 1314 (s), 1275 (s), 1143 (s), 1088 (s), 1041 (s), 941 (m), 916 (m), 849 (s), 792 (m), 759 (w), 740 (w), 698 (m), 656 (w) cm⁻¹. Anal. calc. for C₁₃H₁₂F₆O₂ (314.22): C 49.69, H 3.85; found: C 49.81, H 3.69. HR-MS (EI): calc. for C₁₃H₁₂O₂F₆: 314.0736; found: 314.0737 [M]⁺.

4-Methoxyphenyl(piperidin-1-yl)methanone

R_f (SiO₂, *n*-heptane/EtOAc = 1/1): 0.23. Yield: 73 %. colorless oil. ¹H NMR (400 MHz, DMSO-*d*₆): δ = 7.32 (d, *J* = 8.9 Hz, 2H, CH), 6.96 (d, *J* = 8.9 Hz, 2H, CH), 3.77 (s, 3H, OCH₃), 3.41 (s (broad), 4H, 2CH₂), 1.64-1.55 (m, 2H, CH₂), 1.48 (s(broad), 4H, 2CH₂). ¹³C NMR (100.6 MHz, CDCl₃): δ = 168.8 (C=O), 160.0 and 128,4 (2C), 128.7 and 113,6 (4CH), 55,2 (OCH₃), 25.6 and 24,1 (3CH₂). MS (EI, 70 eV): *m/z* (%) = 218 (41) [M-1]⁺, 135 (100) [OMePhCO]⁺, 92 (19), 77 (25), no other peaks > 10%. IR (KBr): $1/\lambda$ = 3000 (w), 2936 (s), 2855 (m), 1629 (s), 1575 (m), 1512 (s), 1432 (s), 1370 (w), 1351 (w), 1276 (s), 1251 (s), 1175 (s), 1109 (m), 1030 (s), 1001 (m), 955 (w), 886 (w), 841 (s), 793 (w), 763 (m), 594 (m) cm⁻¹. HR-MS (EI): calc. for C₁₃H₁₆NO₂: 218.11756; found: 218.11689 [M-1]⁺.