

Supporting information

Sonogashira Cross-coupling Reactions Catalysed by Copper-free Palladium-zeolites

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Data for the synthesised organic compounds **3-9**:

1-Methoxy-4-phenylethynyl-benzene **3** (R = *p*-OCH₃). Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 70/30. R_f = 0.34. 67% as yellow solid. m.p.: 62.8-63.1 °C.

¹H NMR (250 MHz, CDCl₃): δ ppm: 7.41 (m, 4H, *m*-OCH₃-C₆H₄ and *o*-C≡C-C₆H₅), 7.22 (m, 3H, *p*-C≡C-C₆H₅ and *m*-C≡C-C₆H₅), 6.79 (d, ³J(H,H) = 9.0 Hz, *o*-OCH₃, C₆H₄), 3.73 (s, 3H, CH₃O).

¹³C NMR (62.9 MHz, CDCl₃): δ ppm: 159.61 (C_q-OCH₃, C₆H₄), 133.06 (*m*-OCH₃, C₆H₄), 132.58 (*o*-C≡C, C₆H₅), 128.32 (*m*-C≡C, C₆H₅), 127.94 (*p*-C≡C, C₆H₅), 123.58 (C_q-C≡C, C₆H₅), 115.36 (C_q-C≡C, C₆H₄), 113.99 (*o*-OCH₃, C₆H₄), 89.38 (C≡C-C₆H₅), 88.07 (C≡C-C₆H₄), 55.29 (CH₃O).

C₁₅H₁₂O: mol. wt.: 208.26 g.mol⁻¹. MS: m/z (%) [M⁺] 208 (100), [M⁺ - CH₃] 193 (45), [M⁺ - CH₃ - OH] 176 (7).

1-Methyl-4-phenylethynyl-benzene **3** (R = CH₃). Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 80/20. R_f = 0.52. 82% as white solid. m.p.: 69.8-70.1 °C.

¹H NMR (250 MHz, CDCl₃): δ ppm: 7.45 (m, 2H, *o*-C≡C-C₆H₅), 7.35 (d, 2H, ³J(H,H) = 8.2 Hz, *m*-NO₂-C₆H₄), 7.28 (m, 2H, *m*-C≡C-C₆H₅), 7.26 (m, 1H, *p*-C≡C-C₆H₅), 7.08 (d, 2H, ³J(H,H) = 8.1 Hz), 2.29 (s, 3H, C₆H₄-CH₃).

¹³C NMR (62.9 MHz, CDCl₃): δ ppm: 138.42 (C_q-CH₃, C₆H₄), 131.58 (*m*-CH₃, C₆H₄ and *o*-C≡C, C₆H₅), 129.17 (*o*-CH₃, C₆H₄), 128.37 (*m*-C≡C, C₆H₅), 128.13 (*p*-C≡C, C₆H₅), 123.53 (C_q-C≡C, C₆H₅), 120.24 (C_q-C≡C, C₆H₄), 89.55 (C≡C-C₆H₄), 88.72 (C≡C-C₆H₅), 21.53 (CH₃).

C₁₃H₁₂: mol. wt.: 192.26 g.mol⁻¹. MS: m/z (%) [M⁺] 192 (100), [M⁺ - CH₃, - H] 176 (2), [M⁺ - CH₂=CH] 165 (12), [M⁺ - C₆H₅] 115 (4).

1-Fluoro-4-phenylethynyl-benzene **3** (R = F). Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 80/20. R_f = 0.55. 87% as white solid. m.p.: 110.8-111.3 °C.

¹H NMR (250 MHz, CDCl₃): δ ppm: 7.44 (m, 4H, *m*-F-C₆H₄ and *o*-C≡C-C₆H₅), 7.26 (m, 3H, *p*-C≡C-C₆H₅ and *m*-C≡C-C₆H₅), 6.96 (*pseudo-t*, ³J(H,H) = 8.7 Hz, *o*-F-C₆H₄).

¹³C NMR (62.9 MHz, CDCl₃): δ ppm: 164.46 (C_q-F, C₆H₄), 133.40 (*m*-F, C₆H₄), 131.54 (*o*-C≡C, C₆H₅), 128.36 (*p*-C≡C, C₆H₅), 128.33 (*m*-C≡C, C₆H₅), 123.06 (C_q-C≡C, C₆H₅), 119.32 (C_q-C≡C, C₆H₄), 115.45 (*o*-F, C₆H₄), 89.00 (C≡C-C₆H₄), 88.26 (C≡C-C₆H₅).

C₁₄H₉F: mol. wt.: 196.22 g.mol⁻¹. MS: m/z (%) [M⁺] 196 (100), [M⁺ - F] 177 (10).

1-Nitro-4-phenylethynyl-benzene **3** (R = NO₂). Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 80/20. R_f = 0.26. 85% as a white crystalline solid. m.p.: 119.8-120.3 °C.

¹H NMR (250 MHz, CDCl₃): δ ppm: 8.13 (d, ³J(H,H) = 8.8 Hz, 2H, *o*-NO₂-C₆H₄), 7.58 (d, ³J(H,H) = 8.8 Hz, 2H, *m*-NO₂-C₆H₄), 7.47 (m, 2H, *o*-C≡C-C₆H₅), 7.31 (m, 3H, *m*-C≡C-C₆H₅ and *p*-C≡C-C₆H₅).

¹³C NMR (62.9 MHz, CDCl₃): δ ppm: 146.95 (C_q-NO₂, C₆H₄), 132.26 (*m*-NO₂, C₆H₄), 130.83 (*o*-C≡C, C₆H₅), 130.25 (C_q-C≡C, C₆H₄), 129.27 (*p*-C≡C, C₆H₅), 128.53 (*m*-C≡C, C₆H₅), 123.63 (*o*-NO₂, C₆H₄), 122.08 (C_q-C≡C, C₆H₅), 94.70 (C≡C-C₆H₄), 87.54 (C≡C-C₆H₅).

C₁₄H₉NO₂: mol. wt.: 223.23 g.mol⁻¹. MS: m/z (%) [M⁺] 223 (100), [M⁺ - OH] 207 (7), [M⁺ - NO] 193 (60), [M⁺ - NO₂] 176 (90).

1-(4-Phenylethynyl-phenyl)-ethanone **3** (R = CH₃CO). Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 60/40. R_f = 0.26. 85% as an orange crystalline solid. m.p.: 99.8-100.2 °C.

¹H NMR (250 MHz, CDCl₃): δ ppm: 7.86 (d, 2H, ³J(H,H) = 8.7 Hz, *o*-COCH₃-C₆H₄) 7.53 (d, 2H, ³J(H,H) = 8.7 Hz, *m*-COCH₃-C₆H₄) 7.46 (m, 2H, *o*-C≡C-C₆H₅), 7.29 (m, 3H, *p*-C≡C-C₆H₅ and *m*-C≡C-C₆H₅), 2.54 (s, 3H, CH₃CO).

¹³C NMR (62.9 MHz, CDCl₃): δ ppm: 197.30 (C=O), 136.15 (C_q-COCH₃, C₆H₄), 131.74 (*o*-C≡C, C₆H₅), 131.68 (*o*-C≡C, C₆H₄), 128.82 (*m*-C≡C, C₆H₅), 128.45 (*o*-COCH₃, C₆H₄), 128.16 (C_q-C≡C, C₆H₄), 122.63 (C_q-C≡C, C₆H₅), 92.72 (C≡C-C₆H₄), 88.63 (C≡C-C₆H₅), 26.61 (CH₃CO).

C₁₆H₁₂O: mol. wt.: 220.27 g.mol⁻¹. MS: m/z (%) [M⁺] 220 (60), [M⁺ - CH₃] 205 (100), [M⁺ - CH₃CO] 176 (50).

1-Nitro-2-phenylethynyl-benzene **3** (R = NO₂). Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 60/40. R_f = 0.76. 89% as an orange oil.

¹H NMR (250 MHz, CDCl₃): δ ppm: 8.06 (dd, 1H, ³J(H,H) = 8.2 Hz and ⁴J(H,H) = 1.25 Hz, *o*-NO₂-C₆H₄), 7.69 (dd, 1H, ³J(H,H) = 7.9 Hz, ⁴J(H,H) = 1.6 Hz, *o*-C≡C-C₆H₄), 7.63 (m, 2H, *o*-C≡C-C₆H₅), 7.56 (td, 1H, ³J(H,H) = 7.8 Hz, ⁴J(H,H) = 1.3 Hz, *p*-NO₂-C₆H₄), 7.45 (*pseudo*-td, 1H, ³J(H,H) = 8.8 Hz, ⁴J(H,H) = 1.6 Hz, *m*-NO₂-C₆H₄), 7.40 (m, 3H, *m*-C≡C-C₆H₅ and *p*-C≡C-C₆H₅).

¹³C NMR (62.9 MHz, CDCl₃): δ ppm: 146.51 (C_q-NO₂, C₆H₄), 134.57 (*p*-NO₂, C₆H₄), 132.89 (*o*-C≡C, C₆H₄), 132.01 (*o*-C≡C, C₆H₅), 129.27 (*p*-C≡C, C₆H₄), 128.60 (*p*-C≡C, C₆H₅), 128.49 (*m*-C≡C, C₆H₅), 124.69 (*o*-NO₂, C₆H₄), 122.38 (C_q-C≡C, C₆H₅), 118.66 (C_q-C≡C, C₆H₄), 97.12 (C≡C-C₆H₅), 84.88 (C≡C-C₆H₄).

C₁₄H₉NO₂: mol. wt.: 223.23 g.mol⁻¹. MS: m/z (%) [M⁺] 223 (10), [M⁺ - OH] 206 (30), [M⁺ - NO] 193 (20), [M⁺ - NO₂] 176 (30), [M⁺ - C₆H₅C≡C, - OH] 105 (100), [M⁺ - C₆H₄NO₂, - C≡C] 77 (80).

1-Methyl-2-phenylethynyl-benzene **3** (R = CH₃). Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 80/20. R_f = 0.47. 67% as a colorless oil.

¹H NMR (250 MHz, CDCl₃): δ ppm: 7.41 (m, 3H, *o*-C≡C-C₆H₄ and *o*-C≡C-C₆H₅), 7.20 (m, 3H, *m*-C≡C-C₆H₅ and *p*-C≡C-C₆H₅), 7.09 (m, 3H, *o*-CH₃-C₆H₄; *m*-CH₃-C₆H₄ and *p*-CH₃-C₆H₄), 2.41 (s, 3H, CH₃).

¹³C NMR (62.9 MHz, CDCl₃): δ ppm: 140.24 (C_q-CH₃, C₆H₄), 131.92 (*o*-C≡C, C₆H₄), 131.59 (*m*-C≡C, C₆H₅), 129.55 (*o*-CH₃, C₆H₄), 128.44 (*o*-C≡C, C₆H₅), 128.39 (*p*-C≡C, C₆H₅), 128.25 (*p*-C≡C, C₆H₄), 125.68 (*p*-CH₃, C₆H₄), 123.63 (C_q-C≡C, C₆H₄), 123.10 (C_q-C≡C, C₆H₅), 93.46 (C≡C-C₆H₄), 88.46 (C≡C-C₆H₅), 20.84 (CH₃).

C₁₃H₁₂: mol. wt.: 192.26 g.mol⁻¹. MS: m/z (%) [M⁺] 192 (100), [M⁺ - CH₃, - H] 176 (10), [M⁺ - C₆H₅] 115 (25).

(Z)-1-(1,4-diphenylbut-1-en-3-yn-2-yl)-4-methylbenzene **4**

Eluant: Petroleum-Ether (40-60)/CH₂Cl₂ = 80/20. R_f = 0.33. 28 % as a microcrystalline slightly yellow compound. m.p. = 88.6 - 90.8 °C.

^1H NMR (250 MHz, CDCl_3): δ ppm: 7.86 (d, $^3J(\text{H,H}) = 8.2$ Hz, 2 H; $o\text{-C}=\text{C}-\text{C}_6\text{H}_4$), 7.71 (m, 2 H; $o\text{-C}\equiv\text{C}-\text{C}_6\text{H}_4$), 7.48 (m, 2 H; $o\text{-C}=\text{C}-\text{C}_6\text{H}_5$), 7.30 (m, 6 H; $m\text{-C}=\text{C}-\text{C}_6\text{H}_5$; $p\text{-C}=\text{C}-\text{C}_6\text{H}_5$; $m\text{-C}\equiv\text{C}-\text{C}_6\text{H}_5$; $p\text{-C}\equiv\text{C}-\text{C}_6\text{H}_5$), 7.15 (m, 3 H; $\text{C}=\text{CH}$; $o\text{-CH}_3-\text{C}_6\text{H}_4$), 2.31 (s, 1 H, CH_3).

^{13}C NMR (62.9 MHz, CDCl_3): δ ppm: 139.80 ($\text{C}_q\text{-CH}_3$, C_6H_4), 138.58 ($\text{C}_q\text{-C}=\text{C}$, C_6H_5), 134.98 ($\text{C}=\text{C}-\text{C}_6\text{H}_5$), 134.10 ($\text{C}_q\text{-C}=\text{C}$, C_6H_4), 131.65 ($o\text{-C}\equiv\text{C}$, C_6H_5), 129.29 ($m\text{-C}=\text{C}$, C_6H_5), 129.20 ($m\text{-C}=\text{C}$, C_6H_4), 128.61 ($o\text{-C}=\text{C}$, C_6H_5), 128.58 ($m\text{-C}\equiv\text{C}$, C_6H_5 ; $p\text{-C}\equiv\text{C}$, C_6H_5), 127.89 ($p\text{-C}=\text{C}$, C_6H_5), 126.55 ($o\text{-C}=\text{C}$, C_6H_4), 123.61 ($\text{C}\equiv\text{C}-\text{C}=\text{C}$), 120.72 ($\text{C}_q\text{-C}\equiv\text{C}$, C_6H_5), 97.00 ($\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$), 89.08 ($\text{C}\equiv\text{C}-\text{C}=\text{C}$), 21.58 (CH_3).

$\text{C}_{23}\text{H}_{18}$: mol. wt.: 294.39 $\text{g}\cdot\text{mol}^{-1}$. MS: m/z (%) [M^+] 294 (100), [$\text{M}^+ - \text{CH}_3$] 279 (75), [$\text{M}^+ - \text{CH}_3 - \text{C}_6\text{H}_4$] 215 (25), [$\text{M}^+ - \text{C}\equiv\text{C} - \text{C}_6\text{H}_5$] 202 (30).

3-Phenyl-2-propyn-1-ol 5.

Eluant $\text{CH}_2\text{Cl}_2/\text{Ethanol} = 90/10$. $R_f = 0.73$. 78% as a colourless oil. ^1H NMR (250 MHz, CDCl_3): δ ppm: 7.43 (m, 2H, $o\text{-C}\equiv\text{C}-\text{C}_6\text{H}_5$), 7.26 (m, 3H, $m\text{-C}=\text{C}-\text{C}_6\text{H}_5$; $p\text{-C}=\text{C}-\text{C}_6\text{H}_5$), 4.48 (s, 2H, CH_2OH), 2.42 (brs, 1H, OH).

^{13}C NMR (62.9 MHz, CDCl_3): δ ppm: 131.69 ($o\text{-C}\equiv\text{C}$, C_6H_5), 128.48 ($p\text{-C}\equiv\text{C}$, C_6H_5), 128.32 ($m\text{-C}\equiv\text{C}$, C_6H_5), 87.29 ($\text{C}\equiv\text{C}-\text{CH}_2\text{OH}$), 85.62 ($\text{C}\equiv\text{C}-\text{CH}_2\text{OH}$), 51.50 (CH_2OH).

$\text{C}_9\text{H}_8\text{O}$: mol. wt.: 132.16 $\text{g}\cdot\text{mol}^{-1}$. MS: m/z (%) [$\text{M}^+ - \text{H}$] 131 (100), [$\text{M}^+ - \text{OH}$] 115 (22), [$\text{M}^+ - \text{CHO}$] 103 (46) [C_6H_5^+] 77 (32).

2-phenylindole 6.

Eluant: Petroleum-Ether (40-60)/ $\text{CH}_2\text{Cl}_2 = 2/1$. $R_f = 0.72$ as a light brown compound.

^1H NMR (CDCl_3 , 250 MHz): 6.84 (s, $-\text{CH}=\text{C}-$, 1 H) ; 7.10 to 7.27 (m, 2H, C_6H_4); 7.30 to 7.50 (m, 4H, C_6H_4 and C_6H_5); 7.61 to 7.72 (m, 3H, C_6H_4 and C_6H_5); 8.34 (broad s, 1H, N-H)

^{13}C NMR (CDCl_3 , 62.9 MHz): 99.56 ($\text{CH}=\text{C}-\text{NH}$); 110.51 ($o\text{-C}-\text{N}$ C_6H_4); 119.86 ($o\text{-C}-\text{C}$ C_6H_4); 129.86 and 120.26 ($m\text{-C}-\text{N}$ C_6H_4); 121.94 ($p\text{-C}-\text{N}$ C_6H_4); 124.74 ($o\text{-C}_6\text{H}_5$); 127.30 ($p\text{-C}_6\text{H}_5$); 128.61 ($m\text{-C}_6\text{H}_5$); 129.73 ($\text{C}_q\text{-C}-\text{C}$ C_6H_4); 132.54 ($\text{C}_q\text{-C}-\text{N}$ C_6H_4); 136.82 ($\text{C}=\text{CH}$); 137.73 (C_q C_6H_5).

$\text{C}_{14}\text{H}_{11}\text{N}$, mol. wt.: 193.25, MS: m/z (%): [M^+] 193 (100) [$\text{M}^+ - \text{CHNH}$] 165 (43) [$\text{M}^+ - \text{NH}-\text{C}-\text{C}_6\text{H}_5$] 89 (22).

2-phenylbenzofuran 7.

Eluant: Petroleum-Ether (40-60)/ $\text{CH}_2\text{Cl}_2 = 30/70$. $R_f = 0.72$ as a slightly brown solid. m.p.: 118.3-120.1°C.

^1H NMR (CDCl_3 , 250 MHz): 7.96 (m, 2H, C_6H_4); 7.65 (m, 2H, $o\text{-C}_6\text{H}_5$); 7.36 (m, 5H, C_6H_4 and C_6H_5); 7.08(d, $^4J(\text{H,H}) = 0.9\text{Hz}$, 1H, $\text{CH}=\text{C}$).

^{13}C NMR (CDCl_3 , 62.9 MHz): 156.00 ($\text{O}-\underline{\text{C}}=\text{CH}$); 154.99 ($\text{Cq}-\text{C}-\text{O}$ C_6H_4); 130.56 ($\text{Cq}-\text{C}=\text{C}$ C_6H_5); 129.33 ($p\text{-C}=\text{C}$ C_6H_5); 128.88 ($m\text{-C}=\text{C}$ C_6H_5); 128.63 ($m\text{-C}-\text{O}$ C_6H_4); 125.02 ($o\text{-C}=\text{C}$ C_6H_5); 124.37 ($\text{Cq}-\text{C}=\text{C}$ C_6H_4); 123.04 ($m\text{-C}=\text{C}$ C_6H_4); 121.02 ($o\text{-C}=\text{C}$ C_6H_4); 111.28 ($o\text{-C}-\text{O}$ C_6H_4); 101.42 ($\text{O}-\text{C}=\underline{\text{C}}\text{H}$).

$\text{C}_{14}\text{H}_{10}\text{O}$, mol. wt.: 194.23, MS: m/z (%): $[\text{M}^+]$ 194 (100) $[\text{M}^+ - \text{CHO}]$ 165 (60).

2-phenyl(5-nitrobenzofuran) 8.

Eluant: Petroleum-Ether (40-60)/ $\text{CH}_2\text{Cl}_2 = 20/80$. $R_f = 0.73$ as a slightly brown solid. m.p.: 188.3-120.1°C.

^1H NMR (CDCl_3 , 250 MHz): 8.35 (brd, $^4J(\text{H,H}) = 1.0$ Hz, 1H, $o\text{-NO}_2$ C_6H_3); 8.11 (dd, $^3J(\text{H,H}) = 8.6$ Hz, $^4J(\text{H,H}) = 2.1$ Hz, 1H, $o\text{-NO}_2$ C_6H_3); 7.85 (d, $^3J(\text{H,H}) = 1.7$ Hz, 1H, $o\text{-C}\equiv\text{C}$ C_6H_5); 7.82 (d, $^3J(\text{H,H}) = 1.2$ Hz, 1H, $o\text{-C}\equiv\text{C}$ C_6H_5); 7.58 (d, $^3J(\text{H,H}) = 8.5$ Hz, 1H, $m\text{-NO}_2$ C_6H_3); 7.42 (m, 3H, $m\text{-C}\equiv\text{C}$ C_6H_5 and $p\text{-C}\equiv\text{C}$ C_6H_5).

^{13}C NMR (CDCl_3 , 62.9 MHz): 161.23 ($\text{O}-\underline{\text{C}}=\text{CH}$); 153.30 ($\text{Cq}-\text{C}-\text{O}$ C_6H_3); 144.61 ($\text{Cq}-\text{NO}_2$ C_6H_3); 135.10 ($\text{Cq}-\text{C}_6\text{H}_5$); 129.90 ($\text{Cq}-\text{C}=\text{C}$ C_6H_3); 128.97 ($m\text{-C}=\text{C}$ C_6H_5); 128.91 ($p\text{-C}=\text{C}$ C_6H_5); 125.39 ($o\text{-C}=\text{C}$ C_6H_5); 120.35 ($m\text{-NO}_2$ C_6H_3); 118.81 ($o\text{-NO}_2$ C_6H_3); 107.45 ($o\text{-C}-\text{O}$ C_6H_3); 101.16 ($\text{O}-\text{C}=\underline{\text{C}}\text{H}$).

$\text{C}_{14}\text{H}_9\text{NO}_3$, mol. wt.: 239.23, MS: m/z (%): $[\text{M}^+]$ 239 (100) $[\text{M}^+ - \text{CHO} - \text{H}]$ 203 (70) $[\text{M}^+ - \text{NO}_2]$ 193 (43) $[\text{M}^+ - \text{NO}_2 - \text{CHO}]$ 165 (49).

4-(Phenylethynyl)-6-methyl-2-pyrone 9.

Eluant: Petroleum-Ether (40-60)/ $\text{CH}_2\text{Cl}_2 = 35/65$. $R_f = 0.71$ as a slightly brown solid. m.p.: 65.3-66.7 °C.

^1H NMR (CDCl_3 , 250 MHz): 7.46 (m, 2H, $o\text{-C}\equiv\text{C}-\text{C}_6\text{H}_5$), 7.33 (m, 3H, $m\text{-C}\equiv\text{C}-\text{C}_6\text{H}_5$ and $p\text{-C}\equiv\text{C}-\text{C}_6\text{H}_5$); 6.23 (s, 1H, $\text{O}-\text{C}(\text{O})-\underline{\text{C}}\text{H}=\text{C}$); 5.98 (s, 1H, $\text{CH}_3-\text{C}-\underline{\text{C}}\text{H}=\text{C}$); 2.18 (s, 3H, CH_3).

^{13}C NMR (CDCl_3 , 62.9 MHz): 162.06 ($\underline{\text{C}}=\text{O}$), 161.96 ($\text{CH}_3\underline{\text{C}}=\text{CH}$), 138.90 ($\text{C}\equiv\text{C}-\text{O}-\underline{\text{C}}=\text{CH}$), 132.06 ($o\text{-C}\equiv\text{C}$, C_6H_5), 129.93 ($p\text{-C}\equiv\text{C}$, C_6H_5), 128.55 ($m\text{-C}\equiv\text{C}$, C_6H_5), 121.13 ($\text{Cq}-\text{C}\equiv\text{C}$, C_6H_5), 114.21 ($\text{O}-\text{C}(\text{O})-\underline{\text{C}}\text{H}-\text{C}(\text{C}\equiv\text{C})$), 105.32 ($\text{CH}_3-\text{C}=\underline{\text{C}}\text{H}-\text{C}(\text{C}\equiv\text{C})$), 98.60 ($\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$), 85.39 ($\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$), 19.79 ($\underline{\text{C}}\text{H}_3$).

$\text{C}_{14}\text{H}_{10}\text{O}_2$, mol. wt.: 210.23, MS: m/z (%): $[\text{M}^+]$ 210 (100) $[\text{M}^+ - \text{CO}]$ 182 (85) $[\text{M}^+ - \text{CO} - \text{CH}_2\text{O}]$ 153 (40) $[\text{M}^+ - \text{CO} - \text{C}_2\text{H}_4\text{O}]$ 139 (52).