

**Reactions of 3-aminoisoxazolo[4,5-*c*]coumarin with benzoyl chloride:
the first example of a preparative 1,2,4-oxadiazole–oxazole rearrangement**

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NMR spectra were recorded for DMSO-*d*₆ solutions of compounds at 500.1 MHz for ¹H and 125.8 MHz for ¹³C.

For **7**: ¹H NMR, δ : 7.45 (td, 1H, H-6, *J* 7.5, 0.9 Hz), 7.48 (d, 1H, H-8, *J* 8.3 Hz), 7.68 (t, 2H, H-3', H-5', *J* 7.6 Hz), 7.76 (t, 1H, H-4', *J* 7.5 Hz), 7.77 (ddd, 1H, H-7, *J* 8.5, 7.3, 1.7 Hz), 8.03 (dd, 1H, H-5, *J* 7.9, 1.5 Hz), 8.23 (d, 2H, H-2', H-6', *J* 7.6 Hz). ¹³C NMR, δ : 92.01 (C³), 115.33 (C^{4a}), 116.58 (C⁸), 123.05 (C^{1'}), 124.27 (C⁵), 124.44 (C⁶), 127.98 (C^{2'}, C^{6'}), 129.60 (C^{3'}, C^{5'}), 133.50 (C^{4'}), 134.18 (C⁷), 153.07 (C^{8a}), 159.09 (C²), 163.28 (NCN), 166.01 (C⁴), 174.50 (OCN). IR (ATR, ZnSe, ν/cm^{-1}): 1741, 1607, 1562, 1494. Found (%): C, 66.35; H, 3.43; N, 9.08. Calc. for C₁₇H₁₀N₂O₄ (%): C, 66.67; H, 3.29; N, 9.15.

For **8**: ¹H NMR, δ : 7.46 (dd, 2H, H-3'', H-5'', *J* 8.2, 7.4 Hz), 7.50 (ddd, 1H, H-6, *J* 7.9, 7.4, 1.0 Hz), 7.62–7.70 (m, 6H, H-8, H-2'–H-6'), 7.84 (tt, 1H, H-4'', *J* 7.4, 1.3 Hz), 7.88 (ddd, 1H, H-7, *J* 8.5, 7.2, 1.5 Hz), 7.93 (dd, 1H, H-5, *J* 7.9, 1.5 Hz), 8.19 (dd, 2H, H-2'', H-6'', *J* 8.3, 1.2 Hz). ¹³C NMR, δ : 106.16 (C³), 115.38 (C^{4a}), 116.80 (C⁸), 122.63 (C^{1'}), 124.76 (C⁵), 125.40 (C⁶), 127.37 (C^{1''}), 127.60 (C^{2'}, C^{6'}), 129.24 (C^{3''}, C^{5''}), 129.35 (C^{3'}, C^{5'}), 130.46 (C^{2''}, C^{6''}), 133.45 (C^{4'}), 134.88 (C^{4''}), 135.16 (C⁷), 152.80 (C^{8a}), 157.32 (C²), 160.13 (C⁴), 162.04 (NCN), 162.75 (OCO), 174.64 (OCN). IR (KBr, ν/cm^{-1}): 1749, 1736, 1608, 1576, 1566. Found (%): C, 70.07; H, 3.19; N, 6.94. Calc. for C₂₄H₁₄N₂O₅ (%): C, 70.24; H, 3.44; N, 6.83.

For **9**: ¹H NMR, δ : 7.50 (td, 1H, H-8, *J* 7.6, 1.0 Hz), 7.56–7.62 (m, 3H, H-6, H-3', H-5'), 7.66–7.71 (m, 2H, H-7, H-4'), 7.84 (dd, 1H, H-9, *J* 7.8, 1.3 Hz), 8.06 (d, 2H, H-2', H-6', *J* 7.6 Hz), 12.40 (br. s, 1H, NH). ¹³C NMR, δ : 110.93 (C^{9a}), 117.14 (C⁶), 120.82 (C⁹), 123.90 (C^{3a}), 125.14 (C⁸), 128.30 (C^{2'}, C^{6'}), 128.61 (C^{3'}, C^{5'}), 131.24 (C⁷), 132.32 (C^{1'}), 132.93 (C^{4'}), 151.80 (C^{9b}), 152.02 (C^{5a}), 155.00 (C^{2/C4}), 155.21 (C^{4/C2}), 164.66 (NCO). IR (ATR, ZnSe, ν/cm^{-1}): 3328, 1741, 1715, 1644, 1609, 1591, 1531. Found (%): C, 66.34; H, 3.34; N, 8.97. Calc. for C₁₇H₁₀N₂O₄ (%): C, 66.67; H, 3.29; N, 9.15.