

Supplementary data for article:

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Supplementary Material

Synthesis, crystal structures and antimicrobial activity of azido and isocyanato Zn(II) complexes with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent

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Synthesis of (E)-N,N,N-trimethyl-2-oxo-2-(2-(quinolin-2-ylmethylene)hydrazinyl)ethan-1-aminium chloride (HLCl)

2-Quinolinecarboxaldehyde 0.31 g (2.00 mmol) was dissolved in ethanol (25 mL) and Girard's T reagent 0.34 g (2.00 mmol) was added. The mixture was refluxed for 3 h. After cooling to the room temperature, a white precipitate was filtered and washed with ethanol. IR (cm⁻¹): 3414 (m), 3062 (m), 2970 (m), 2939 (m), 2831 (m), 1699 (s), 1595 (m), 1562 (w), 1497 (m), 1414 (m), 1379 (w), 1340 (w), 1301 (m), 1230 (m), 1135 (m), 989 (w), 950 (w), 916 (w), 868 (w), 832 (w), 758 (m), 656 (w), 633 (w), 533 (w).

¹H NMR (500 MHz, CD₃OD), (numbering of atoms according to Scheme 1), δ (ppm) 3.47 (s, 9H, C12-H), 4.94 (s, 2H, C11-H), 8.17 (s, 1H, C9-H), 8.18 (d, 1H, ³J_{C3-H/C4-H} = 10 Hz, C3-H), 8.36 (d, 1H, ³J_{C3-H/C4-H} = 10 Hz, C4-H), 7.94 (d, 1H, ³J_{C5-H/C6-H} = 5 Hz, C5-H), 7.62 (t, 1H, ³J_{C5-H/C6-H/C7-H} = 5 Hz, C6-H), 7.78 (t, 1H, ³J_{C6-H/C7-H/C8-H} = 5 Hz, C7-H), 8.03 (d, 1H, ³J_{C7-H/C8-H} = 5 Hz, C8-H).

¹³C NMR (125 MHz, CD₃OD), (numbering of atoms according to scheme 1), δ (ppm) 55.0 (C12), 64.4 (C11), 146.9 (C9), 154.4 (C2), 119.2 (C3), 138.7 (C4), 130.1 (C4a), 129.3 (C5), 129.0 (C6), 131.7 (C7), 129.7 (C8), 148.9 (C8a), 167.0 (C10).