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Synthesis and crystal structure of benzyl 5-oxo-5-phenyl-2-(quinolin-2-yl)pentanoate, C₂₇H₂₃NO₃

Table 2 (continued)

Atom	x	y	z	U _{iso} [*] /U _{eq}
C18	0.8078(4)	0.48159(18)	0.1055(2)	0.0282(6)
H18	0.9509	0.4545	0.1039	0.034*
C19	0.6314(4)	0.54257(17)	0.6421(2)	0.0263(6)
H19A	0.5715	0.5464	0.7260	0.032*
H19B	0.7757	0.5742	0.6460	0.032*
C20	0.4541(4)	0.57852(16)	0.5412(2)	0.0225(5)
H20A	0.5345	0.5965	0.4684	0.027*
H20B	0.3425	0.5365	0.5101	0.027*
C21	0.3230(4)	0.64851(17)	0.5896(2)	0.0247(5)
C22	0.1205(4)	0.68145(17)	0.5059(2)	0.0225(5)
C23	−0.0255(4)	0.73535(18)	0.5593(2)	0.0278(6)
H23	0.0062	0.7504	0.6458	0.033*
C24	−0.2158(5)	0.76690(19)	0.4870(3)	0.0330(6)
H24	−0.3138	0.8037	0.5236	0.040*
C25	−0.2634(4)	0.74450(19)	0.3604(3)	0.0300(6)
H25	−0.3938	0.7661	0.3105	0.036*
C26	−0.1212(5)	0.69096(19)	0.3073(3)	0.0303(6)
H26	−0.1541	0.6757	0.2210	0.036*
C27	0.0698(4)	0.65917(18)	0.3796(2)	0.0272(6)
H27	0.1663	0.6220	0.3426	0.033*
N1	0.7677(3)	0.36043(14)	0.78520(19)	0.0236(5)
O1	0.9648(3)	0.47657(14)	0.46326(17)	0.0365(5)
O2	0.6493(3)	0.40280(12)	0.40803(16)	0.0283(4)
O3	0.3745(3)	0.67556(15)	0.69553(17)	0.0383(5)

0.01 mmol), [1,1'-biphenyl]-3,3',5,5'-tetracarboxylic acid (3.30 mg, 0.01 mmol) and zinc(II) acetate dihydrate (2.19 mg, 0.01 mmol) were dissolved in DMF and aqueous solution (8 mL) in a 10 mL vial, which was heated at 433.15 K for 72 h to produce clear light colourless crystals. Elemental analysis supports the composition of the title compound. **Anal.** **Calcd.** for C₂₇H₂₃NO₃: C, 79.20%; H, 5.66%; N, 3.42%. **Found:** C, 79.49%; H, 5.51%; N, 3.21%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Esters are considered to be a very important class of organic compounds and have broad application prospects [4, 5]. More esters have been synthesized, but their practical application is not sufficient, and more researchers are needed to focus their interest on the application of such compounds in order to achieve progress. The title compound introduces a quinoline group into the ester, which increases the coordination

point and fluorescent properties. For example: for medical drug research [6, 7], organic synthesis reactions [8], luminescences [9], molecular sensors [10, 11] and so on.

The crystal structure is only built up by C₂₇H₂₃NO₃ molecules. In the molecules, there is a pair of intramolecular C—H···O hydrogen bonds (C20—H20B···O1: d(C20—H20B) = 0.99 Å, d(H20B···O1) = 2.42 Å, d(C20···O1) = 3.349(3) Å) and the geometric parameters are in expected ranges [12].

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