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# (*E*)-3-(2-Ethoxyquinolin-3-yl)-1-(2-hydroxy-6-methylphenyl)prop-2-en-1-one

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**Key indicators**

Single-crystal X-ray study
*T* = 296 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.033
*wR* factor = 0.085
Data-to-parameter ratio = 7.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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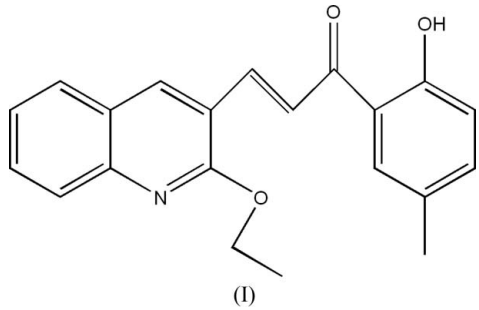
The title molecule, $C_{21}H_{19}NO_3$, consists of a 2-ethoxyquinolyl group linked to an aroylvinyl group. The quinolyl ring forms a dihedral angle of 2.88 (6)° with the benzene ring. The crystal structure can be described by two types of crossed layers which are parallel to (110) and (1$\bar{1}$0). The packing is stabilized by C—H···O and O—H···O intra- and intermolecular hydrogen bonds, resulting in the formation of a two-dimensional network.

## Comment

Heterocycles such as indole, pyrimidine, pyridine and quinoline are an integral part of a large number of natural and synthetic compounds which play important roles in many biological systems (Sundberg, 1996; Fritz *et al.*, 2001). As a structural subunit in many natural products, the quinoline ring system is one of the most commonly encountered heterocycles in medicinal chemistry. A literature survey revealed that substituted quinolines possess diverse chemotherapeutic activities including antibacterial (Kayirere *et al.*, 1998, Kidwai *et al.*, 2000), antifungal (Musiol *et al.*, 2006), anti-amoebic (Burkhaller & Edgerton, 1951; Bailey *et al.*, 1979), anti-leishmanial (Dade *et al.*, 2001; Jain *et al.*, 2005), antimalarial (Charris *et al.*, 2005; Cunico *et al.*, 2006) and antitumor activities (Zhao *et al.*, 2005; Chen *et al.*, 2006). Furthermore, heterocyclic chalcone analogs, act as intermediate products in the synthesis of practically important flavonoids and themselves show useful biological activity (Dhar & Barton, 1981). Molecules of these compounds are conformationally mobile, hence, a series of investigations has been concerned with a study of their three-dimensional structure (Khilya *et al.*, 1991; Bologa *et al.*, 1989; Furmanova *et al.*, 1991). In the course of our ongoing program related to the synthesis and the biological evaluation of new quinoline derivatives (Lalaoui *et al.*, 2003; Menasra *et al.*, 2005; Belfaitah *et al.*, 2006; Bouraiou *et al.*, 2007), we report here the synthesis and crystal structure of the title compound, (I).




(I)

The molecular structure of (I), which consists of a 2-ethoxyquinolyl unit linked to an aroylvinyl group, is shown in

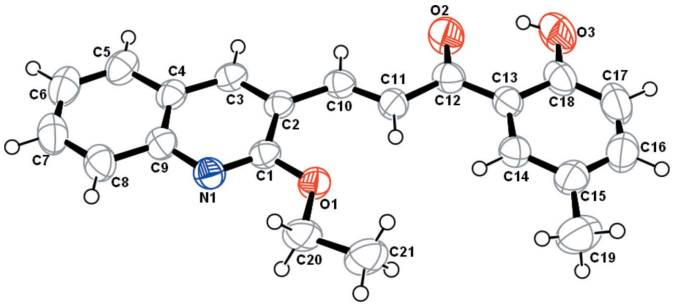



**Figure 1**
The molecular structure of (I), with the atomic labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

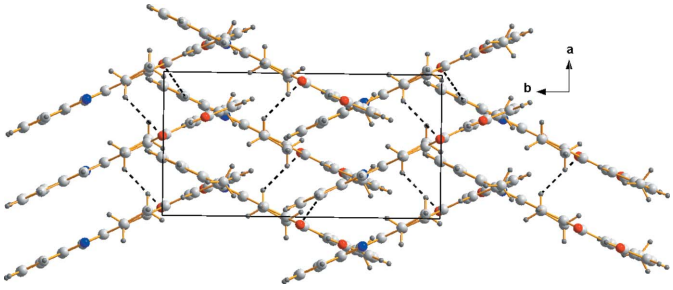



**Figure 2**
View of the layered crystal packing of (I). Hydrogen bonds are shown as dashed lines.

Fig. 1. The two rings of the quinolyl unit form a dihedral angle of 0.64 (8)° and this unit forms a dihedral angle of 2.88 (6)° with the benzene ring. The geometric parameters of (I) (Table 1) are in agreement with those of other structures possessing a quinolyl substituent previously reported in the literature (Belfaitah *et al.*, 2006; Bouraiou *et al.*, 2007).

The crystal structure can be described by two types of crossed layers, parallel to (110) and (1$\bar{1}$0) (Fig. 2). The packing is stabilized by C—H···O and O—H···O intra- and intermolecular hydrogen bonds, resulting in the formation of a two-dimensional network (Fig. 2). Hydrogen-bonding parameters are listed in (Table 2).

## Experimental

The title compound was synthesized by refluxing 2-chloro-3-formylquinoline (2.61 mmol) and 2-hydroxy-5-methylphenylacetophenone (2.61 mmol) in ethanol (15 ml) in the presence of NaOH (50%, 13 mmol) for 24 h. The contents were then cooled and poured into cold water and acidified with dilute HCl (5 ml, 1 *N*). A yellow solid was obtained that was filtered off, washed and dried to afford the crude chalcone. Crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane solution of (I).

*Crystal data*

$C_{21}H_{19}NO_3$
$M_r$ = 333.37
Orthorhombic, $Pn2_1a$
$a$ = 7.6026 (2) Å
$b$ = 14.7425 (4) Å
$c$ = 15.6862 (4) Å
$V$ = 1758.13 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 296 (2) K
0.15 × 0.11 × 0.06 mm

*Data collection*

Bruker–Nonius KappaCCD diffractometer
Absorption correction: none
24253 measured reflections
1869 independent reflections
1348 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.085
$S$ = 1.03
1869 reflections
236 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.12 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C1 | 1.356 (3) | O3—C18 | 1.349 (3) |
| O1—C20 | 1.444 (2) | N1—C1 | 1.302 (3) |
| O2—C12 | 1.249 (3) | N1—C9 | 1.375 (3) |
| | | | |
| C1—O1—C20 | 117.53 (18) | N1—C9—C4 | 121.9 (2) |
| C1—N1—C9 | 118.00 (18) | O2—C12—C11 | 120.0 (2) |
| O1—C1—N1 | 118.71 (17) | O2—C12—C13 | 120.4 (2) |
| N1—C1—C2 | 125.4 (2) | O3—C18—C13 | 121.8 (2) |
| O1—C1—C2 | 115.87 (19) | O3—C18—C17 | 119.0 (3) |
| N1—C9—C8 | 119.0 (2) | O1—C20—C21 | 106.80 (19) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H33···O2 | 0.82 | 1.81 | 2.541 (3) | 147 |
| C3—H3···O3$^{i}$ | 0.93 | 2.56 | 3.441 (3) | 159 |
| C10—H10···O2 | 0.93 | 2.44 | 2.801 (3) | 103 |
| C11—H11···O1 | 0.93 | 2.19 | 2.813 (3) | 124 |

Symmetry code: (i) $-x, y+\frac{1}{2}, -z+1$.

All H atoms were localized in Fourier maps but introduced in calculated positions and treated as riding on their parent C atom with C—H = 0.93–0.97 Å, O—H = 0.82 and $U_{iso}$(H) = 1.2–1.5$U_{eq}$(carrier atom). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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