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Ethyl 5-chloro-9-ethoxy-2-oxo-2*H*-pyrano-[2,3-*g*]quinoline-8-carboxylate

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The title compound, $C_{17}H_{14}ClNO_5$ has been shown to be isostructural with the bromo analogue, confirming the site of alkylation within the structure and the pyranoquinoline ring system. As with the bromo analogue, the molecules are linked by a C—H···O hydrogen bond forming *C*(5) chains along [001].

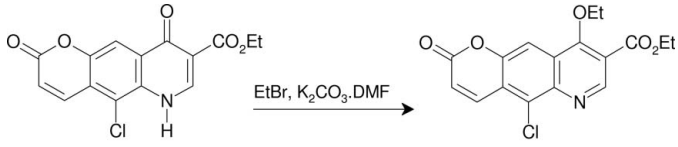
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.052
wR factor = 0.076
Data-to-parameter ratio = 22.9

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

Comment

Following from the successful bromination of a pyranoquinoline derivative (da Matta *et al.*, 2000; de Oliveira, 2003) at the carbonyl site of compound (1) (see scheme) (de Oliveira, 2006), chlorination was also attempted. As with the bromo compound (de Oliveira *et al.*, 2006), alkylation occurs at the carbonyl site (Fig. 1).



(1) (2)

The structure also reveals the same hydrogen bonding scheme with intramolecular hydrogen bonds (Table 1) supporting the structure, and *C*(5) chains (Bernstein *et al.*, 1995) forming along [001] (de Oliveira *et al.*, 2006).

Experimental

The title compound was obtained from the reaction between EtBr and (1) in DMF solution in the presence of K_2CO_3 (de Oliveira,

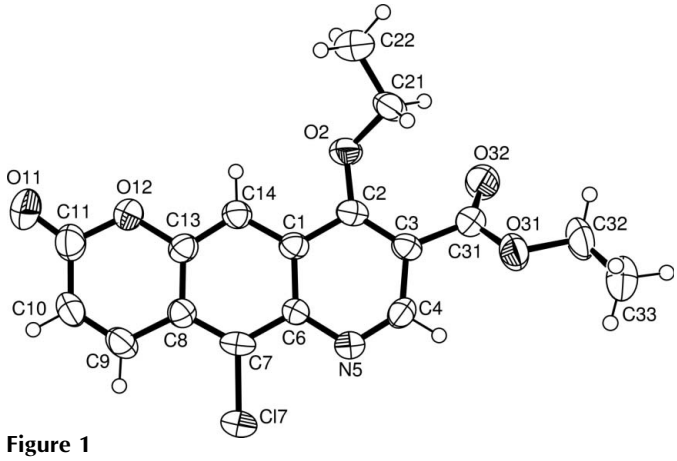


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

2003). Pure product (2) was obtained from the reaction mixture by column chromatography using hexane–ethyl acetate as the eluent (gradient 1:4 to 1:1). Crystals suitable for X-ray crystallography were grown from ethyl acetate (65% yield; m.p. 433–434 K).

Crystal data

$C_{17}H_{14}ClNO_5$
M_r = 347.74
Orthorhombic, $Pna2_1$
a = 7.1480 (9) Å
b = 19.653 (3) Å
c = 11.1150 (14) Å
V = 1561.4 (3) Å^3
Z = 4
D_x = 1.479 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1346 reflections
θ = 3.5–19.3°
μ = 0.27 mm^{-1}
T = 291 (2) K
Needle, colourless
0.38 × 0.10 × 0.02 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.866, T_{max} = 0.995
15310 measured reflections
5017 independent reflections
1745 reflections with $I > 2\sigma(I)$
R_{int} = 0.100
θ_{max} = 32.5°
$h = -10 \rightarrow 10$
$k = -29 \rightarrow 29$
$l = -16 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.076
S = 0.79
5017 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0131P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 2061 Friedel pairs
Flack parameter: 0.00 (7)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O11^{i}	0.93	2.55	3.357 (4)	145
C4—H4···O31	0.93	2.40	2.730 (4)	101
C9—H9···Cl7	0.93	2.71	3.071 (3)	104
C21—H21*A*···O32	0.97	2.30	2.927 (4)	122

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

All H atoms were located in difference maps and then treated as riding atoms, with C—H distances of 0.95 (aromatic) or 0.96 Å (methyl) and U_{iso}(H) values of $1.2U_{eq}$(C) (aromatic) or $1.5U_{eq}$(C) (methyl). *PLATON* (Spek, 2003) was used for the hydrogen-bonding analysis.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CIFTAB* (Sheldrick, 1997).

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Acta Cryst. (2006). E**62**, o1494–o1495 [https://doi.org/10.1107/S160053680600715X]

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Cell parameters from 1346 reflections
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$h = -10\rightarrow10$
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Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.076$
$S = 0.79$
5017 reflections
219 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0131P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.00 (7)

Special details

Experimental. IR (KBr, cm^{-1}): 2979, 1749, 1718, 1618, 1590, 1342, 1302. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 1.51 (*t*, *J* = 7.2 Hz, 3H), 1.59 (*t*, *J* = 6.9 Hz, 3H), 4.46 (*q*, *J* = 6.9 Hz, 2H), 4.56 (*q*, *J* = 7.2 Hz, 2H), 6.93 (*d*, *J* = 9.9 Hz, 1H), 8.18 (*s*, 1H), 8.57 (*d*, *J* = 9.9 Hz, 1H), 9.25 (*s*, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz): δ 13.9, 15.3, 61.7, 72.3, 107.2, 115.1, 120.3, 121.0, 125.3, 131.5, 139.4, 142.5, 150.3, 151.9, 158.5, 162.2, 164.3.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5477 (4)	0.26739 (15)	0.7928 (2)	0.0384 (8)
C2	0.5707 (5)	0.32697 (15)	0.8673 (2)	0.0396 (9)
O2	0.6140 (3)	0.31280 (9)	0.98103 (16)	0.0554 (6)
C21	0.7298 (5)	0.35674 (14)	1.0542 (3)	0.0515 (9)
H21A	0.6546	0.3921	1.0911	0.062*
H21B	0.8259	0.3780	1.0054	0.062*
C22	0.8169 (5)	0.31246 (17)	1.1489 (3)	0.0742 (11)
H22A	0.7203	0.2894	1.1929	0.111*
H22B	0.8887	0.3401	1.2031	0.111*
H22C	0.8972	0.2796	1.1114	0.111*
C3	0.5482 (4)	0.38991 (15)	0.8139 (3)	0.0394 (8)
C31	0.5414 (5)	0.45618 (17)	0.8800 (3)	0.0492 (9)
O31	0.6132 (4)	0.50542 (10)	0.81272 (17)	0.0627 (7)
O32	0.4740 (3)	0.46481 (10)	0.9783 (2)	0.0691 (7)
C32	0.5921 (6)	0.57510 (16)	0.8570 (3)	0.0734 (12)
H32A	0.6493	0.5799	0.9357	0.088*
H32B	0.4608	0.5871	0.8632	0.088*
C33	0.6887 (5)	0.61997 (15)	0.7671 (3)	0.0808 (13)
H33A	0.8192	0.6086	0.7642	0.121*
H33B	0.6745	0.6667	0.7906	0.121*
H33C	0.6340	0.6133	0.6891	0.121*
C4	0.5045 (4)	0.39197 (14)	0.6895 (3)	0.0448 (9)
H4	0.4947	0.4348	0.6544	0.054*
N5	0.4765 (4)	0.33948 (13)	0.6193 (2)	0.0460 (7)
C6	0.4954 (4)	0.27698 (14)	0.6713 (2)	0.0383 (7)
C7	0.4651 (4)	0.21757 (16)	0.6005 (2)	0.0430 (8)
Cl7	0.39837 (12)	0.22796 (4)	0.45262 (8)	0.0614 (2)
C8	0.4881 (4)	0.15307 (15)	0.6457 (3)	0.0403 (8)
C9	0.4591 (4)	0.09056 (16)	0.5782 (3)	0.0516 (9)
H9	0.4179	0.0926	0.4989	0.062*
C10	0.4911 (5)	0.03104 (17)	0.6289 (3)	0.0591 (10)
H10	0.4684	−0.0082	0.5843	0.071*

C11	0.5598 (5)	0.02387 (17)	0.7506 (3)	0.0586 (10)
O11	0.6028 (4)	−0.02798 (11)	0.8000 (2)	0.0799 (9)
O12	0.5750 (3)	0.08350 (10)	0.81648 (17)	0.0533 (6)
C13	0.5440 (4)	0.14710 (14)	0.7658 (3)	0.0417 (8)
C14	0.5745 (4)	0.20186 (14)	0.8390 (2)	0.0417 (8)
H14	0.6123	0.1957	0.9183	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.040 (2)	0.0420 (19)	0.0329 (17)	−0.0042 (16)	0.0025 (14)	0.0021 (15)
C2	0.037 (2)	0.049 (2)	0.0322 (18)	−0.0073 (16)	−0.0010 (14)	0.0006 (15)
O2	0.0779 (18)	0.0508 (13)	0.0374 (14)	−0.0159 (12)	−0.0108 (12)	0.0064 (10)
C21	0.060 (3)	0.055 (2)	0.039 (2)	−0.0083 (18)	−0.0076 (16)	−0.0096 (15)
C22	0.094 (3)	0.075 (2)	0.054 (2)	0.000 (2)	−0.022 (2)	0.0072 (18)
C3	0.042 (2)	0.045 (2)	0.0313 (18)	−0.0024 (15)	0.0027 (15)	−0.0029 (14)
C31	0.060 (3)	0.043 (2)	0.045 (2)	0.0036 (19)	−0.0045 (18)	0.0000 (17)
O31	0.094 (2)	0.0416 (14)	0.0527 (14)	−0.0067 (14)	0.0116 (12)	−0.0089 (11)
O32	0.102 (2)	0.0574 (14)	0.0482 (17)	0.0106 (14)	0.0127 (15)	−0.0039 (11)
C32	0.104 (3)	0.040 (2)	0.076 (3)	0.001 (2)	0.005 (2)	−0.0202 (18)
C33	0.108 (4)	0.043 (2)	0.091 (3)	−0.003 (2)	−0.002 (3)	−0.002 (2)
C4	0.051 (2)	0.0366 (18)	0.047 (2)	0.0034 (17)	−0.0014 (16)	0.0078 (16)
N5	0.056 (2)	0.0437 (16)	0.0382 (16)	0.0017 (13)	−0.0065 (13)	0.0011 (13)
C6	0.047 (2)	0.0358 (18)	0.0323 (16)	−0.0019 (16)	−0.0014 (14)	−0.0012 (15)
C7	0.038 (2)	0.063 (2)	0.0277 (16)	−0.0005 (17)	−0.0046 (14)	−0.0009 (15)
Cl7	0.0839 (7)	0.0643 (5)	0.0361 (4)	0.0005 (5)	−0.0135 (5)	−0.0033 (4)
C8	0.041 (2)	0.0401 (19)	0.0400 (19)	−0.0002 (16)	0.0013 (15)	−0.0015 (15)
C9	0.063 (3)	0.052 (2)	0.0397 (19)	−0.0050 (19)	0.0057 (17)	−0.0111 (16)
C10	0.083 (3)	0.042 (2)	0.053 (2)	−0.003 (2)	−0.001 (2)	−0.0132 (17)
C11	0.070 (3)	0.043 (2)	0.062 (3)	−0.003 (2)	0.004 (2)	−0.0017 (19)
O11	0.110 (3)	0.0407 (16)	0.0885 (18)	0.0019 (16)	−0.0146 (16)	0.0038 (14)
O12	0.0716 (18)	0.0401 (13)	0.0482 (13)	−0.0033 (13)	−0.0040 (12)	0.0032 (10)
C13	0.044 (2)	0.041 (2)	0.0396 (19)	−0.0001 (16)	0.0024 (16)	0.0050 (15)
C14	0.045 (2)	0.0415 (19)	0.0383 (17)	−0.0061 (16)	−0.0019 (15)	0.0011 (15)

Geometric parameters (Å, º)

C1—C14	1.400 (3)	C33—H33A	0.9600
C1—C6	1.414 (4)	C33—H33B	0.9600
C1—C2	1.444 (4)	C33—H33C	0.9600
C2—O2	1.331 (3)	C4—N5	1.309 (3)
C2—C3	1.381 (4)	C4—H4	0.9300
O2—C21	1.446 (3)	N5—C6	1.364 (3)
C21—C22	1.501 (4)	C6—C7	1.425 (3)
C21—H21A	0.9700	C7—C8	1.373 (4)
C21—H21B	0.9700	C7—Cl7	1.724 (3)
C22—H22A	0.9600	C8—C13	1.399 (4)
C22—H22B	0.9600	C8—C9	1.454 (4)

C22—H22C	0.9600	C9—C10	1.318 (4)
C3—C4	1.418 (4)	C9—H9	0.9300
C3—C31	1.497 (4)	C10—C11	1.446 (4)
C31—O32	1.206 (3)	C10—H10	0.9300
C31—O31	1.326 (3)	C11—O11	1.198 (3)
O31—C32	1.463 (3)	C11—O12	1.386 (3)
C32—C33	1.500 (4)	O12—C13	1.389 (3)
C32—H32A	0.9700	C13—C14	1.367 (3)
C32—H32B	0.9700	C14—H14	0.9300

C14—C1—C6	120.6 (3)	H33A—C33—H33B	109.5
C14—C1—C2	121.3 (3)	C32—C33—H33C	109.5
C6—C1—C2	118.0 (3)	H33A—C33—H33C	109.5
O2—C2—C3	128.5 (3)	H33B—C33—H33C	109.5
O2—C2—C1	113.7 (3)	N5—C4—C3	126.3 (3)
C3—C2—C1	117.8 (3)	N5—C4—H4	116.8
C2—O2—C21	122.8 (2)	C3—C4—H4	116.8
O2—C21—C22	106.6 (2)	C4—N5—C6	116.2 (3)
O2—C21—H21A	110.4	N5—C6—C1	123.4 (3)
C22—C21—H21A	110.4	N5—C6—C7	119.3 (3)
O2—C21—H21B	110.4	C1—C6—C7	117.3 (3)
C22—C21—H21B	110.4	C8—C7—C6	122.4 (3)
H21A—C21—H21B	108.6	C8—C7—Cl7	119.4 (2)
C21—C22—H22A	109.5	C6—C7—Cl7	118.2 (2)
C21—C22—H22B	109.5	C7—C8—C13	117.4 (3)
H22A—C22—H22B	109.5	C7—C8—C9	125.0 (3)
C21—C22—H22C	109.5	C13—C8—C9	117.5 (3)
H22A—C22—H22C	109.5	C10—C9—C8	120.3 (3)
H22B—C22—H22C	109.5	C10—C9—H9	119.8
C2—C3—C4	118.1 (3)	C8—C9—H9	119.8
C2—C3—C31	124.9 (3)	C9—C10—C11	123.0 (3)
C4—C3—C31	116.6 (3)	C9—C10—H10	118.5
O32—C31—O31	124.3 (3)	C11—C10—H10	118.5
O32—C31—C3	125.5 (3)	O11—C11—O12	117.2 (3)
O31—C31—C3	110.2 (3)	O11—C11—C10	126.8 (3)
C31—O31—C32	117.0 (2)	O12—C11—C10	116.0 (3)
O31—C32—C33	106.2 (2)	C11—O12—C13	122.3 (2)
O31—C32—H32A	110.5	C14—C13—O12	116.2 (3)
C33—C32—H32A	110.5	C14—C13—C8	123.2 (3)
O31—C32—H32B	110.5	O12—C13—C8	120.5 (3)
C33—C32—H32B	110.5	C13—C14—C1	119.0 (3)
H32A—C32—H32B	108.7	C13—C14—H14	120.5
C32—C33—H33A	109.5	C1—C14—H14	120.5
C32—C33—H33B	109.5		

C14—C1—C2—O2	−1.5 (4)	C2—C1—C6—C7	−177.2 (3)
C6—C1—C2—O2	177.9 (3)	N5—C6—C7—C8	177.6 (3)
C14—C1—C2—C3	177.8 (3)	C1—C6—C7—C8	−1.2 (4)

C6—C1—C2—C3	−2.8 (4)	N5—C6—C7—Cl7	−2.0 (4)
C3—C2—O2—C21	−31.0 (5)	C1—C6—C7—Cl7	179.2 (2)
C1—C2—O2—C21	148.2 (3)	C6—C7—C8—C13	−0.2 (5)
C2—O2—C21—C22	−154.9 (3)	Cl7—C7—C8—C13	179.4 (2)
O2—C2—C3—C4	179.0 (3)	C6—C7—C8—C9	179.9 (3)
C1—C2—C3—C4	−0.2 (4)	Cl7—C7—C8—C9	−0.5 (4)
O2—C2—C3—C31	−9.4 (5)	C7—C8—C9—C10	177.7 (3)
C1—C2—C3—C31	171.4 (3)	C13—C8—C9—C10	−2.2 (4)
C2—C3—C31—O32	−34.8 (6)	C8—C9—C10—C11	−1.6 (5)
C4—C3—C31—O32	136.9 (4)	C9—C10—C11—O11	−175.1 (4)
C2—C3—C31—O31	148.0 (3)	C9—C10—C11—O12	5.6 (5)
C4—C3—C31—O31	−40.3 (4)	O11—C11—O12—C13	174.6 (3)
O32—C31—O31—C32	−5.9 (5)	C10—C11—O12—C13	−6.1 (4)
C3—C31—O31—C32	171.3 (3)	C11—O12—C13—C14	−176.3 (3)
C31—O31—C32—C33	178.5 (3)	C11—O12—C13—C8	2.6 (4)
C2—C3—C4—N5	2.5 (5)	C7—C8—C13—C14	0.6 (5)
C31—C3—C4—N5	−169.8 (3)	C9—C8—C13—C14	−179.5 (3)
C3—C4—N5—C6	−1.4 (5)	C7—C8—C13—O12	−178.2 (3)
C4—N5—C6—C1	−1.9 (5)	C9—C8—C13—O12	1.7 (4)
C4—N5—C6—C7	179.3 (3)	O12—C13—C14—C1	179.3 (3)
C14—C1—C6—N5	−176.6 (3)	C8—C13—C14—C1	0.4 (5)
C2—C1—C6—N5	4.0 (5)	C6—C1—C14—C13	−1.8 (4)
C14—C1—C6—C7	2.2 (4)	C2—C1—C14—C13	177.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O11^{i}	0.93	2.55	3.357 (4)	145
C4—H4···O31	0.93	2.40	2.730 (4)	101
C9—H9···Cl7	0.93	2.71	3.071 (3)	104
C21—H21*A*···O32	0.97	2.30	2.927 (4)	122

Symmetry code: (i) −*x*+1, −*y*, *z*−1/2.