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# 3-[(*E*)-1-(Benzyloxyimino)ethyl]-7-(3-methylbut-2-enyloxy)-2*H*-chromen-2-one

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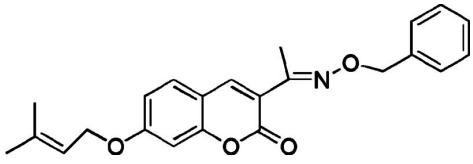
Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.052; $wR$ factor = 0.155; data-to-parameter ratio = 15.2.

In the title compound, $C_{23}H_{23}NO_4$, the dihedral angle beween the chromen-2-one ring system and the benzene ring is 69.73 (10)° and the molecule adopts an *E* conformation with respect to the C=N double bond. In the crystal, inversion dimers linked by pairs of C—H···O hydrogen bonds occur, generating $R_2^2(12)$ loops.

## Related literature

For background to the use of Schiff bases as chemosensors, see: Li *et al.* (2009).



## Experimental

### Crystal data

$C_{23}H_{23}NO_4$ $M_r$ = 377.42
Triclinic, $P\overline{1}$
$a$ = 7.3038 (19) Å
$b$ = 11.467 (3) Å
$c$ = 12.184 (3) Å
$\alpha$ = 92.368 (3)°
$\beta$ = 92.067 (3)°
$\gamma$ = 102.340 (3)°
$V$ = 995.0 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 273 K
0.26 × 0.18 × 0.16 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.978, $T_{max}$ = 0.986
5604 measured reflections
3912 independent reflections
2341 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.155
$S$ = 1.01
3912 reflections
257 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8···O2$^{i}$ | 0.93 | 2.43 | 3.338 (3) | 167 |

Symmetry code: (i) $-x, -y, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5875).

## References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, H. Y., Gao, S. & Xi, Z. (2009). *Inorg. Chem. Commun.* **12**, 300–303.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supplementary materials

*Acta Cryst.* (2011). E**67**, o1516 [ **doi:10.1107/S1600536811019015** ]

# 3-[(*E*)-1-(Benzyloxyimino)ethyl]-7-(3-methylbut-2-enyloxy)-2*H*-chromen-2-one

**H. Wang, L. He, W. Zheng and H. Song**

## Comment

Coumarin-derived Schiff bases have attracted attention as colorimetric chemosensors (Li *et al.*, 2009). Herein, we report the crystal structure of the title compound, (I), Fig. 1, obtained by the reaction of 3-acetyl-7-(3-methylbut-2-enyloxy)-2*H*-chromen-2-one with benzyloxy-amine. Inversion dimers occur in the crystal, being linked by pairs of C—H···O hydrogen bonds (Table 1).

## Experimental

A mixture of 3-acetyl-7-(3-methylbut-2-enyloxy)-2*H*-chromen-2-one (1 mmol) and benzyloxy- amine hydrochloride (1.2 mmol) in ethanol (15 ml) was heated at 313 K for 0.5 h, the solution pH was then maintained at a value of 7 by the addition of sodium carbonate(0.5 mmol). The reaction mixture was refluxed for 10 h at 333 K (monitored by TLC). After completion of the reaction, the solvent was removed under a vacuum. The crude product was purified by chromatography (ethyl acetate: petroleum ether = 3:1). The eluate was evaporated to give the title compound as colourless blocks (279 mg, 74%; m. p. 372–374 K). ESI-MS (m / *z*): [(*M*+Na)+] 400, [(*M*+H)+] 378; IR (KBr, cm-1) 3065, 2971, 2877, 1722, 1603, 1491, 1458, 1357, 1259, 1216, 1129, 981, 923, 772; 1H NMR(400 MHz, CDCl3, TMS) delta 7.79 (s, 1H), 7.40 (d, 1H, J = 8.4 Hz), 7.31–7.36 (m, 5H), 6.83 (dd, 1H, J = 2.8, 8.4 Hz), 6.79(d 1H, J = 2.8 Hz), 5.45–5.50 (m, 1H), 5.23 (s, 2H), 4.56(d, 2H, J = 6.8 Hz), 2.27 (s, 3H), 1.80 (s, 3H), 1.76 (s, 3H); 13 C NMR (100 MHz, CDCl3) delta 162.45, 160.08, 155.90, 154.33, 141.40, 137.72, 129.49, 128.96, 128.41, 128.33, 127.97, 127.84,127.42, 121.30, 118.59, 113.57, 112.43, 101.08, 76.21, 65.46, 25.83,18.30,14.61.

## Figures

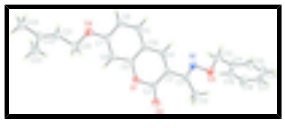

Fig. 1. The molecular structure of the title compound showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

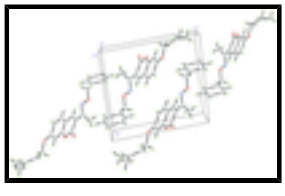

Fig. 2. Crystal packing in the title compound.

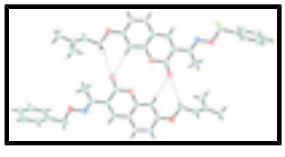

Fig. 3. Part of the crystal structure of the title compound showing weak C—H···O hydrogen bonds as dashed lines.

Fig. 4. The formation of the title compound.

### 3-[(*E*)-1-(Benzyloxyimino)ethyl]-7-(3-methylbut-2-enyloxy)- 2*H*-chromen-2-one

*Crystal data*

| | |
|---|---|
| $C_{23}H_{23}NO_4$ | $Z = 2$ |
| $M_r = 377.42$ | $F(000) = 430.0$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.260$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.3038$ (19) Å | Cell parameters from 1391 reflections |
| $b = 11.467$ (3) Å | $\theta = 2.4$–$24.9°$ |
| $c = 12.184$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $\alpha = 92.368$ (3)° | $T = 273$ K |
| $\beta = 92.067$ (3)° | Block, colorless |
| $\gamma = 102.340$ (3)° | 0.26 × 0.18 × 0.16 mm |
| $V = 995.0$ (5) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 3912 independent reflections |
| Radiation source: fine-focus sealed tube | 2341 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.032$ |
| φ and ω scans | $\theta_{max} = 26.3°$, $\theta_{min} = 1.8°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2004) | $h = -9 \rightarrow 8$ |
| $T_{min} = 0.978$, $T_{max} = 0.986$ | $k = -10 \rightarrow 14$ |
| 5604 measured reflections | $l = -14 \rightarrow 15$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.052$ | H-atom parameters constrained |
| $wR(F^2) = 0.155$ | $w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.1016P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.01$ | $(\Delta/\sigma)_{max} = 0.028$ |
| 3912 reflections | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 257 parameters | $\Delta\rho_{min} = -0.19$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.049 (5) |

*Special details*

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.4410 (2) | 0.43803 (16) | 0.26381 (14) | 0.0548 (5) |
| O3 | 0.59306 (19) | 0.46642 (13) | 0.19438 (12) | 0.0611 (4) |
| O2 | 0.3010 (2) | 0.10766 (13) | 0.38943 (12) | 0.0622 (4) |
| O1 | 0.04470 (18) | 0.14660 (12) | 0.45666 (10) | 0.0492 (4) |
| O4 | −0.50894 (19) | 0.21552 (13) | 0.61925 (11) | 0.0558 (4) |
| C19 | 0.9868 (3) | 0.6503 (2) | 0.19649 (18) | 0.0627 (6) |
| H19 | 0.9821 | 0.6483 | 0.2726 | 0.075* |
| C18 | 1.1555 (3) | 0.6776 (2) | 0.1505 (2) | 0.0776 (8) |
| H18 | 1.2648 | 0.6934 | 0.1952 | 0.093* |
| C17 | 1.1667 (4) | 0.6820 (3) | 0.0413 (3) | 0.0852 (9) |
| H17 | 1.2835 | 0.7011 | 0.0107 | 0.102* |
| C16 | 1.0072 (5) | 0.6584 (3) | −0.0255 (2) | 0.0898 (9) |
| H16 | 1.0149 | 0.6616 | −0.1014 | 0.108* |
| C15 | 0.8327 (4) | 0.6296 (2) | 0.0215 (2) | 0.0743 (7) |
| H15 | 0.7235 | 0.6132 | −0.0232 | 0.089* |
| C14 | 0.8222 (3) | 0.62545 (18) | 0.13341 (18) | 0.0539 (6) |
| C13 | 0.6388 (4) | 0.5931 (2) | 0.1861 (3) | 0.0872 (9) |
| H13B | 0.6471 | 0.6325 | 0.2587 | 0.105* |
| H13A | 0.5422 | 0.6184 | 0.1423 | 0.105* |
| C11 | 0.3842 (3) | 0.32488 (19) | 0.26814 (16) | 0.0485 (5) |
| C12 | 0.4680 (4) | 0.2348 (2) | 0.2070 (2) | 0.0742 (7) |
| H12C | 0.5063 | 0.2642 | 0.1369 | 0.111* |
| H12A | 0.3765 | 0.1611 | 0.1961 | 0.111* |
| H12B | 0.5750 | 0.2214 | 0.2486 | 0.111* |
| C3 | 0.2208 (3) | 0.28938 (17) | 0.33767 (15) | 0.0449 (5) |
| C2 | 0.1984 (3) | 0.17731 (18) | 0.39329 (15) | 0.0462 (5) |
| C9 | −0.0825 (3) | 0.21796 (17) | 0.47168 (14) | 0.0418 (5) |
| C4 | 0.0943 (3) | 0.35857 (18) | 0.35299 (15) | 0.0481 (5) |
| H4 | 0.1091 | 0.4300 | 0.3175 | 0.058* |
| C10 | −0.0610 (3) | 0.32596 (17) | 0.42160 (15) | 0.0437 (5) |
| C5 | −0.1943 (3) | 0.39482 (19) | 0.44254 (17) | 0.0530 (5) |
| H5 | −0.1839 | 0.4680 | 0.4104 | 0.064* |
| C6 | −0.3389 (3) | 0.35666 (19) | 0.50912 (17) | 0.0529 (5) |

| | | | | |
|---|---|---|---|---|
| H6 | −0.4246 | 0.4042 | 0.5231 | 0.064* |
| C8 | −0.2289 (3) | 0.17562 (18) | 0.53828 (15) | 0.0460 (5) |
| H8 | −0.2400 | 0.1022 | 0.5699 | 0.055* |
| C7 | −0.3581 (3) | 0.24560 (18) | 0.55642 (15) | 0.0458 (5) |
| C20 | −0.5503 (3) | 0.0961 (2) | 0.65844 (17) | 0.0564 (6) |
| H20B | −0.4576 | 0.0878 | 0.7150 | 0.068* |
| H20A | −0.5481 | 0.0381 | 0.5985 | 0.068* |
| C21 | −0.7401 (3) | 0.07576 (19) | 0.70411 (16) | 0.0536 (5) |
| H21 | −0.8390 | 0.0794 | 0.6550 | 0.064* |
| C22 | −0.7839 (3) | 0.05328 (19) | 0.80605 (16) | 0.0516 (5) |
| C24 | −0.6452 (4) | 0.0473 (3) | 0.89720 (19) | 0.0908 (9) |
| H24C | −0.5213 | 0.0617 | 0.8696 | 0.136* |
| H24A | −0.6738 | −0.0304 | 0.9268 | 0.136* |
| H24B | −0.6510 | 0.1069 | 0.9539 | 0.136* |
| C23 | −0.9843 (3) | 0.0309 (2) | 0.8392 (2) | 0.0740 (7) |
| H23B | −1.0643 | 0.0390 | 0.7770 | 0.111* |
| H23C | −0.9965 | 0.0879 | 0.8969 | 0.111* |
| H23A | −1.0200 | −0.0484 | 0.8648 | 0.111* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0458 (10) | 0.0545 (12) | 0.0642 (11) | 0.0066 (9) | 0.0195 (8) | 0.0119 (9) |
| O3 | 0.0547 (9) | 0.0495 (10) | 0.0799 (10) | 0.0063 (7) | 0.0285 (8) | 0.0151 (7) |
| O2 | 0.0598 (9) | 0.0552 (10) | 0.0791 (10) | 0.0235 (8) | 0.0188 (8) | 0.0198 (8) |
| O1 | 0.0493 (8) | 0.0467 (9) | 0.0545 (8) | 0.0125 (7) | 0.0135 (6) | 0.0161 (6) |
| O4 | 0.0584 (9) | 0.0500 (9) | 0.0602 (9) | 0.0102 (7) | 0.0212 (7) | 0.0094 (7) |
| C19 | 0.0675 (15) | 0.0652 (16) | 0.0569 (13) | 0.0157 (13) | 0.0105 (11) | 0.0086 (11) |
| C18 | 0.0535 (15) | 0.089 (2) | 0.0876 (19) | 0.0105 (14) | 0.0042 (13) | 0.0007 (15) |
| C17 | 0.0681 (18) | 0.089 (2) | 0.096 (2) | 0.0059 (15) | 0.0369 (16) | 0.0044 (16) |
| C16 | 0.122 (3) | 0.093 (2) | 0.0524 (15) | 0.0134 (19) | 0.0287 (17) | 0.0138 (14) |
| C15 | 0.0760 (18) | 0.0710 (18) | 0.0716 (16) | 0.0083 (14) | −0.0149 (13) | 0.0084 (13) |
| C14 | 0.0487 (13) | 0.0434 (13) | 0.0715 (14) | 0.0097 (10) | 0.0176 (11) | 0.0137 (10) |
| C13 | 0.0692 (17) | 0.0507 (16) | 0.150 (3) | 0.0176 (13) | 0.0500 (17) | 0.0331 (16) |
| C11 | 0.0480 (12) | 0.0480 (13) | 0.0491 (11) | 0.0080 (10) | 0.0081 (9) | 0.0058 (9) |
| C12 | 0.0839 (18) | 0.0575 (16) | 0.0832 (17) | 0.0131 (13) | 0.0391 (14) | 0.0051 (13) |
| C3 | 0.0458 (11) | 0.0430 (12) | 0.0453 (10) | 0.0064 (9) | 0.0075 (8) | 0.0072 (9) |
| C2 | 0.0449 (11) | 0.0469 (13) | 0.0467 (11) | 0.0082 (10) | 0.0057 (9) | 0.0072 (9) |
| C9 | 0.0435 (11) | 0.0416 (12) | 0.0412 (10) | 0.0108 (9) | 0.0031 (8) | 0.0047 (8) |
| C4 | 0.0508 (12) | 0.0435 (12) | 0.0489 (11) | 0.0060 (10) | 0.0046 (9) | 0.0111 (9) |
| C10 | 0.0431 (11) | 0.0433 (12) | 0.0436 (10) | 0.0059 (9) | 0.0032 (8) | 0.0075 (9) |
| C5 | 0.0536 (13) | 0.0454 (13) | 0.0616 (13) | 0.0110 (10) | 0.0085 (10) | 0.0146 (10) |
| C6 | 0.0519 (12) | 0.0448 (13) | 0.0649 (13) | 0.0144 (10) | 0.0097 (10) | 0.0085 (10) |
| C8 | 0.0511 (12) | 0.0427 (12) | 0.0436 (10) | 0.0069 (10) | 0.0064 (9) | 0.0084 (9) |
| C7 | 0.0465 (11) | 0.0465 (12) | 0.0425 (10) | 0.0042 (9) | 0.0101 (8) | 0.0046 (9) |
| C20 | 0.0637 (14) | 0.0540 (14) | 0.0522 (12) | 0.0108 (11) | 0.0156 (10) | 0.0106 (10) |
| C21 | 0.0486 (12) | 0.0603 (14) | 0.0501 (12) | 0.0054 (10) | 0.0072 (9) | 0.0111 (10) |
| C22 | 0.0539 (13) | 0.0507 (13) | 0.0490 (11) | 0.0066 (10) | 0.0091 (9) | 0.0062 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.0810 (19) | 0.136 (3) | 0.0548 (14) | 0.0192 (18) | 0.0014 (13) | 0.0171 (15) |
| C23 | 0.0656 (16) | 0.0839 (19) | 0.0709 (16) | 0.0066 (14) | 0.0209 (12) | 0.0184 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C11 | 1.279 (3) | C3—C4 | 1.354 (3) |
| N1—O3 | 1.4111 (19) | C3—C2 | 1.459 (3) |
| O3—C13 | 1.428 (3) | C9—C8 | 1.382 (2) |
| O2—C2 | 1.207 (2) | C9—C10 | 1.385 (3) |
| O1—C9 | 1.375 (2) | C4—C10 | 1.428 (3) |
| O1—C2 | 1.377 (2) | C4—H4 | 0.9300 |
| O4—C7 | 1.356 (2) | C10—C5 | 1.402 (3) |
| O4—C20 | 1.443 (2) | C5—C6 | 1.363 (3) |
| C19—C18 | 1.353 (3) | C5—H5 | 0.9300 |
| C19—C14 | 1.373 (3) | C6—C7 | 1.401 (3) |
| C19—H19 | 0.9300 | C6—H6 | 0.9300 |
| C18—C17 | 1.338 (3) | C8—C7 | 1.381 (3) |
| C18—H18 | 0.9300 | C8—H8 | 0.9300 |
| C17—C16 | 1.368 (4) | C20—C21 | 1.488 (3) |
| C17—H17 | 0.9300 | C20—H20B | 0.9700 |
| C16—C15 | 1.396 (4) | C20—H20A | 0.9700 |
| C16—H16 | 0.9300 | C21—C22 | 1.316 (3) |
| C15—C14 | 1.371 (3) | C21—H21 | 0.9300 |
| C15—H15 | 0.9300 | C22—C24 | 1.490 (3) |
| C14—C13 | 1.488 (3) | C22—C23 | 1.504 (3) |
| C13—H13B | 0.9700 | C24—H24C | 0.9600 |
| C13—H13A | 0.9700 | C24—H24A | 0.9600 |
| C11—C3 | 1.483 (3) | C24—H24B | 0.9600 |
| C11—C12 | 1.495 (3) | C23—H23B | 0.9600 |
| C12—H12C | 0.9600 | C23—H23C | 0.9600 |
| C12—H12A | 0.9600 | C23—H23A | 0.9600 |
| C12—H12B | 0.9600 | | |
| C11—N1—O3 | 111.18 (16) | O1—C9—C10 | 120.44 (16) |
| N1—O3—C13 | 108.13 (15) | C8—C9—C10 | 123.15 (18) |
| C9—O1—C2 | 123.03 (15) | C3—C4—C10 | 122.46 (18) |
| C7—O4—C20 | 117.49 (15) | C3—C4—H4 | 118.8 |
| C18—C19—C14 | 121.5 (2) | C10—C4—H4 | 118.8 |
| C18—C19—H19 | 119.2 | C9—C10—C5 | 117.12 (17) |
| C14—C19—H19 | 119.2 | C9—C10—C4 | 117.73 (18) |
| C17—C18—C19 | 120.6 (3) | C5—C10—C4 | 125.15 (18) |
| C17—C18—H18 | 119.7 | C6—C5—C10 | 121.29 (19) |
| C19—C18—H18 | 119.7 | C6—C5—H5 | 119.4 |
| C18—C17—C16 | 120.4 (2) | C10—C5—H5 | 119.4 |
| C18—C17—H17 | 119.8 | C5—C6—C7 | 119.89 (19) |
| C16—C17—H17 | 119.8 | C5—C6—H6 | 120.1 |
| C17—C16—C15 | 119.2 (2) | C7—C6—H6 | 120.1 |
| C17—C16—H16 | 120.4 | C7—C8—C9 | 118.06 (18) |
| C15—C16—H16 | 120.4 | C7—C8—H8 | 121.0 |
| C14—C15—C16 | 120.1 (2) | C9—C8—H8 | 121.0 |

| | | | |
|---|---|---|---|
| C14—C15—H15 | 119.9 | O4—C7—C8 | 124.63 (18) |
| C16—C15—H15 | 119.9 | O4—C7—C6 | 114.90 (17) |
| C15—C14—C19 | 118.1 (2) | C8—C7—C6 | 120.47 (18) |
| C15—C14—C13 | 121.5 (2) | O4—C20—C21 | 107.58 (17) |
| C19—C14—C13 | 120.3 (2) | O4—C20—H20B | 110.2 |
| O3—C13—C14 | 108.12 (18) | C21—C20—H20B | 110.2 |
| O3—C13—H13B | 110.1 | O4—C20—H20A | 110.2 |
| C14—C13—H13B | 110.1 | C21—C20—H20A | 110.2 |
| O3—C13—H13A | 110.1 | H20B—C20—H20A | 108.5 |
| C14—C13—H13A | 110.1 | C22—C21—C20 | 127.4 (2) |
| H13B—C13—H13A | 108.4 | C22—C21—H21 | 116.3 |
| N1—C11—C3 | 113.69 (18) | C20—C21—H21 | 116.3 |
| N1—C11—C12 | 124.18 (19) | C21—C22—C24 | 124.4 (2) |
| C3—C11—C12 | 122.1 (2) | C21—C22—C23 | 121.23 (19) |
| C11—C12—H12C | 109.5 | C24—C22—C23 | 114.42 (18) |
| C11—C12—H12A | 109.5 | C22—C24—H24C | 109.5 |
| H12C—C12—H12A | 109.5 | C22—C24—H24A | 109.5 |
| C11—C12—H12B | 109.5 | H24C—C24—H24A | 109.5 |
| H12C—C12—H12B | 109.5 | C22—C24—H24B | 109.5 |
| H12A—C12—H12B | 109.5 | H24C—C24—H24B | 109.5 |
| C4—C3—C2 | 118.98 (17) | H24A—C24—H24B | 109.5 |
| C4—C3—C11 | 122.25 (18) | C22—C23—H23B | 109.5 |
| C2—C3—C11 | 118.75 (17) | C22—C23—H23C | 109.5 |
| O2—C2—O1 | 116.02 (17) | H23B—C23—H23C | 109.5 |
| O2—C2—C3 | 126.66 (18) | C22—C23—H23A | 109.5 |
| O1—C2—C3 | 117.31 (17) | H23B—C23—H23A | 109.5 |
| O1—C9—C8 | 116.41 (16) | H23C—C23—H23A | 109.5 |

*Hydrogen-bond geometry (°)*

*D*—H···*A*

—···

**Fig. 1**

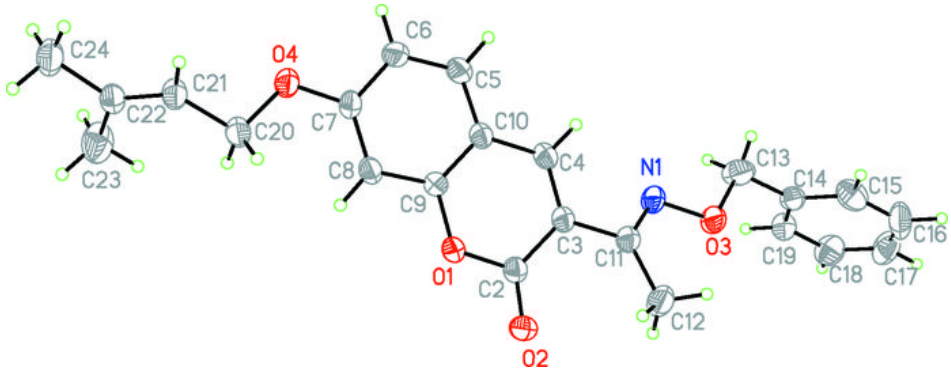
C24
C22
C23
C21
O4
C20
C6
C5
C7
C10
C8
C4
C9
N1
C13
C14
C15
C16
C3
C11
O3
C19
C18
C17
O1
C2
C12
O2

**Fig. 2**

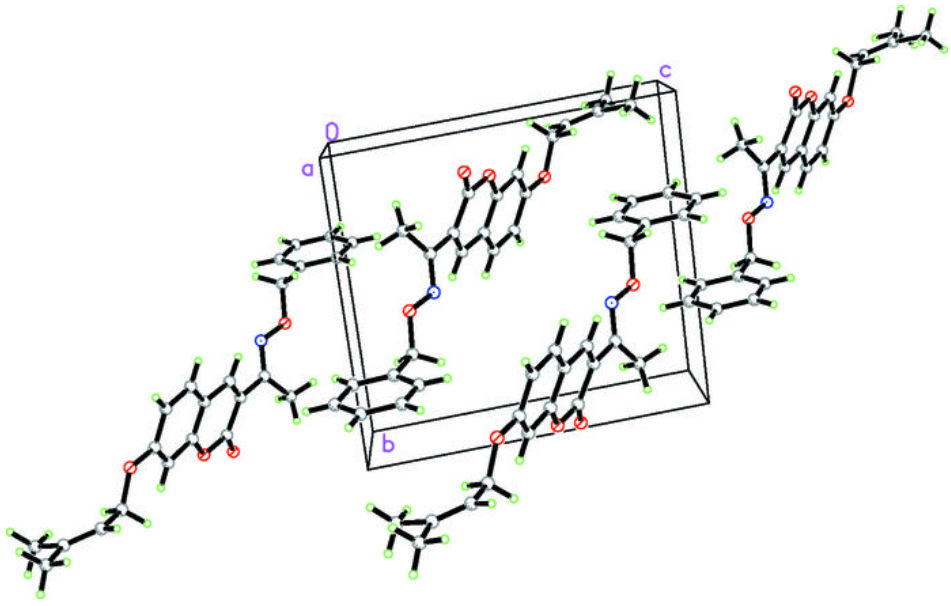

**Fig. 3**

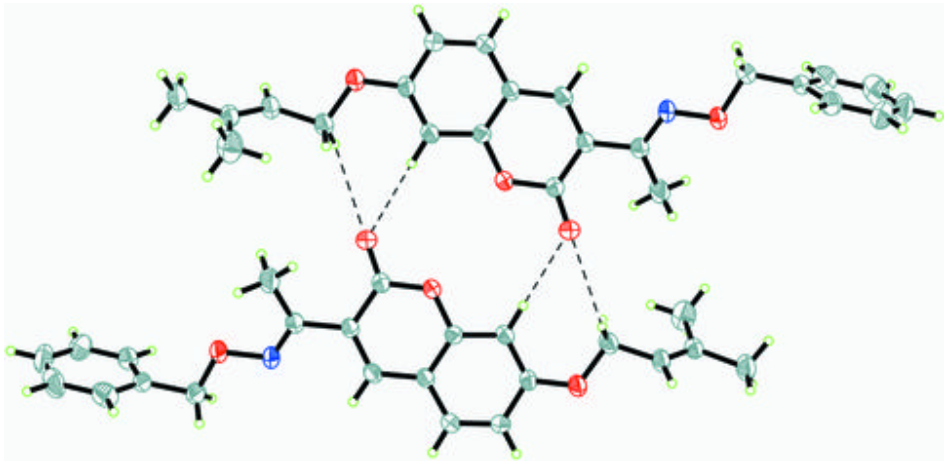

**Fig. 4**