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(*S*)-Ethyl 2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy]propanoate

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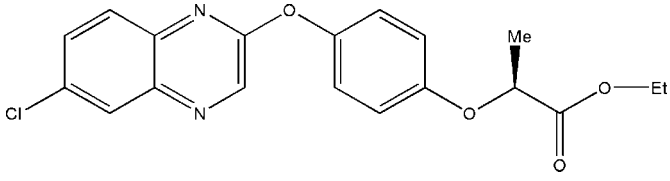
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.155; data-to-parameter ratio = 8.1.

In the molecule of the title compound, $C_{19}H_{17}ClN_2O_4$, the quinoxaline ring system is planar [maximum deviation = 0.013 (3) Å] and oriented at a dihedral angle of 80.18 (3)° with respect to the benzene ring. In the crystal structure, intermolecular C—H···N interactions link molecules into chains. π–π contacts between the quinoxaline systems [centroid–centroid distance = 3.654 (1) Å] may further stabilize the structure.

Related literature

The title compound has potent selective herbicidal activity against annual and perennial grass weeds, see: Sakata *et al.* (1985). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{19}H_{17}ClN_2O_4$ M_r = 372.80
Monoclinic, $P2_1$
a = 9.970 (2) Å
b = 4.4760 (9) Å
c = 20.450 (4) Å
β = 94.54 (3)°
V = 909.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 294 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.932, T_{max} = 0.977
3762 measured reflections
1898 independent reflections
1254 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.155
S = 1.00
1898 reflections
235 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 932 Friedel pairs
Flack parameter: −0.02 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19A···N1^{i}	0.93	2.57	3.396 (7)	149

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2712).

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supplementary materials

Acta Cryst. (2009). E**65**, o2082 [**doi:10.1107/S1600536809030074**]

(*S*)-Ethyl 2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy]propanoate

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Comment

The title compound has a potent selective herbicidal activity against annual and perennial grass weeds (Sakata *et al.*, 1985). We report herein its crystal structure.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C6-C11), B (C13-C18) and C (N1/N2/C12/C13/C18/C19) are, of course, planar, and they are oriented at dihedral angles of A/B = 80.21 (3), A/C = 80.07 (3) and B/C = 0.66 (3) °. The quinoxaline ring system is planar with a maximum deviation of -0.013 (3) Å for atom N1.

In the crystal structure, intermolecular C-H···N interactions link the molecules into chains (Fig. 2), in which they may be effective in the stabilization of the structure. The π–π contact between the quinoxaline rings, Cg2—Cg3^{i} [symmetry code: (i) x, y - 1, z, where Cg2 and Cg3 are centroids of the rings B (C13-C18) and C (N1/N2/C12/C13/C18/C19), respectively] may further stabilize the structure, with centroid-centroid distance of 3.654 (1) Å.

Experimental

For the preparation of the title compound, thionyl chloride (3.7 ml, 50 mmol) was added in dropwise to (*S*)-2-(4-(6-chloroquinoxalin-2-yloxy)phenoxy)propanoate acid (3.72 g, 10 mmol) in an ice bath (263 K). After refluxing for 5 h, the mixture was cooled to room temperature, and excess thionyl chloride was removed by reduced pressure distillation. Then, the residue was dissolved in a solution of ethanol (4.9 ml, 80 mmol) and pyridine (2.5 ml, 30 mmol). The solid residue was extracted with hexane (40 ml) and hexane was distilled off. Crystals suitable for X-ray analysis were formed after 8 d in ethyl acetate by slow evaporation at room temperature.

Refinement

H atoms were positioned geometrically with C-H = 0.93, 0.98, 0.97 and 0.96 Å, for aromatic, methine, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H and x = 1.2 for aromatic H atoms.

Figures

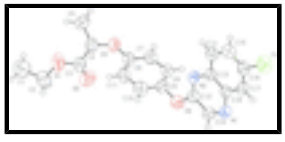

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

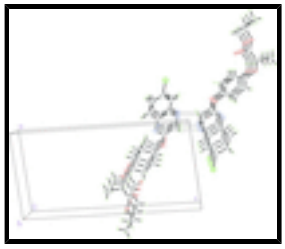

Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

(*S*)-Ethyl 2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy]propanoate

Crystal data

$C_{19}H_{17}ClN_2O_4$	F_{000} = 388
M_r = 372.80	D_x = 1.361 Mg m^{-3}
Monoclinic, $P2_1$	Melting point: 350 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 9.970 (2) Å	Cell parameters from 25 reflections
b = 4.4760 (9) Å	θ = 9–12º
c = 20.450 (4) Å	μ = 0.24 mm^{-1}
β = 94.54 (3)º	T = 294 K
V = 909.7 (3) Å^3	Needle, colorless
Z = 2	0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.052
Radiation source: fine-focus sealed tube	θ_{max} = 25.4º
Monochromator: graphite	θ_{min} = 2.0º
T = 294 K	h = −11→11
ω/2θ scans	k = −5→0
Absorption correction: ψ scan (North *et al.*, 1968)	l = −24→24
T_{min} = 0.932, T_{max} = 0.977	3 standard reflections
3762 measured reflections	every 120 min
1898 independent reflections	intensity decay: 1%
1254 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.050	$w = 1/[\sigma^2(F_o^2) + (0.085P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.155	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.17 e Å^{-3}

1898 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}
235 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 932 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.02 (18)
Secondary atom site location: difference Fourier map	

Special details

Experimental. 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 $F^2 > 2\text{sigma}(F^2)$ 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.

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}
Cl	0.50826 (14)	0.9066 (5)	0.08796 (7)	0.0921 (6)
O1	1.8615 (3)	0.4503 (12)	0.3878 (2)	0.0925 (14)
O2	1.7523 (4)	0.0871 (12)	0.3367 (2)	0.0956 (14)
O3	1.5198 (3)	0.2389 (10)	0.38949 (16)	0.0730 (11)
O4	1.2147 (3)	0.1148 (12)	0.15458 (16)	0.0838 (13)
N1	0.9132 (4)	0.2496 (12)	0.05649 (17)	0.0616 (11)
N2	1.0378 (4)	0.4196 (12)	0.18081 (17)	0.0563 (10)
C1	2.0926 (5)	0.474 (2)	0.4119 (4)	0.131 (3)
H1B	2.1793	0.4138	0.3993	0.196*
H1C	2.0803	0.3998	0.4551	0.196*
H1D	2.0871	0.6882	0.4120	0.196*
C2	1.9882 (5)	0.353 (2)	0.3656 (3)	0.095 (2)
H2B	1.9988	0.4282	0.3218	0.115*
H2C	1.9928	0.1370	0.3648	0.115*
C3	1.7536 (5)	0.3000 (15)	0.3698 (3)	0.0657 (15)
C4	1.6313 (4)	0.4380 (16)	0.3988 (2)	0.0710 (15)
H4A	1.6092	0.6308	0.3779	0.085*
C5	1.6551 (6)	0.476 (2)	0.4726 (3)	0.107 (3)
H5A	1.5771	0.5645	0.4893	0.161*
H5B	1.7316	0.6029	0.4824	0.161*
H5C	1.6716	0.2841	0.4927	0.161*
C6	1.4468 (4)	0.2317 (14)	0.3298 (2)	0.0582 (13)

C7	1.3386 (5)	0.0408 (14)	0.3263 (2)	0.0656 (14)
H7A	1.3203	−0.0682	0.3633	0.079*
C8	1.2570 (5)	0.0074 (15)	0.2696 (2)	0.0715 (17)
H8A	1.1837	−0.1217	0.2677	0.086*
C9	1.2861 (5)	0.1681 (15)	0.2160 (2)	0.0637 (15)
C10	1.3937 (5)	0.3564 (15)	0.2181 (3)	0.0720 (15)
H10A	1.4119	0.4639	0.1808	0.086*
C11	1.4758 (5)	0.3883 (16)	0.2752 (3)	0.0718 (15)
H11A	1.5500	0.5147	0.2765	0.086*
C12	1.0919 (5)	0.2395 (14)	0.1409 (2)	0.0612 (13)
C13	0.9127 (4)	0.5295 (12)	0.1580 (2)	0.0517 (12)
C14	0.8466 (5)	0.7268 (13)	0.1979 (2)	0.0586 (13)
H14A	0.8859	0.7811	0.2389	0.070*
C15	0.7228 (5)	0.8395 (14)	0.1757 (2)	0.0658 (15)
H15A	0.6783	0.9715	0.2017	0.079*
C16	0.6646 (5)	0.7562 (14)	0.1148 (2)	0.0626 (14)
C17	0.7261 (5)	0.5646 (14)	0.0749 (2)	0.0614 (14)
H17A	0.6852	0.5136	0.0340	0.074*
C18	0.8516 (4)	0.4457 (12)	0.0964 (2)	0.0509 (12)
C19	1.0293 (5)	0.1538 (15)	0.0790 (2)	0.0646 (15)
H19A	1.0746	0.0216	0.0534	0.078*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0714 (9)	0.1061 (14)	0.0958 (11)	0.0193 (10)	−0.0124 (7)	0.0154 (11)
O1	0.056 (2)	0.079 (3)	0.141 (3)	−0.003 (2)	0.003 (2)	−0.029 (3)
O2	0.092 (3)	0.083 (3)	0.111 (3)	0.010 (3)	0.002 (2)	−0.037 (3)
O3	0.063 (2)	0.087 (3)	0.067 (2)	−0.018 (2)	−0.0070 (16)	0.000 (2)
O4	0.065 (2)	0.115 (4)	0.070 (2)	0.028 (3)	−0.0046 (17)	−0.022 (2)
N1	0.061 (2)	0.071 (3)	0.051 (2)	−0.001 (3)	−0.0001 (18)	0.002 (2)
N2	0.054 (2)	0.066 (3)	0.049 (2)	0.001 (2)	−0.0021 (16)	−0.001 (2)
C1	0.062 (4)	0.123 (8)	0.205 (8)	0.012 (5)	−0.004 (4)	−0.024 (7)
C2	0.066 (3)	0.099 (5)	0.123 (5)	0.013 (4)	0.016 (3)	0.007 (5)
C3	0.061 (3)	0.067 (4)	0.068 (3)	0.001 (3)	−0.003 (2)	0.000 (3)
C4	0.055 (3)	0.067 (4)	0.089 (4)	−0.005 (3)	−0.004 (2)	−0.014 (3)
C5	0.078 (4)	0.156 (8)	0.087 (4)	−0.006 (5)	0.001 (3)	−0.055 (5)
C6	0.048 (2)	0.064 (3)	0.063 (3)	−0.002 (3)	0.004 (2)	−0.006 (3)
C7	0.058 (3)	0.074 (4)	0.064 (3)	−0.009 (3)	0.004 (2)	−0.001 (3)
C8	0.054 (3)	0.091 (5)	0.070 (3)	−0.010 (3)	0.009 (2)	−0.013 (3)
C9	0.051 (3)	0.077 (4)	0.062 (3)	0.014 (3)	−0.004 (2)	−0.016 (3)
C10	0.073 (3)	0.070 (4)	0.072 (3)	0.002 (3)	0.002 (3)	0.008 (3)
C11	0.061 (3)	0.074 (4)	0.080 (3)	−0.017 (3)	−0.002 (2)	0.011 (4)
C12	0.060 (3)	0.070 (4)	0.053 (3)	0.000 (3)	0.002 (2)	0.002 (3)
C13	0.052 (2)	0.056 (3)	0.047 (2)	−0.007 (2)	−0.0007 (19)	0.005 (2)
C14	0.061 (3)	0.057 (3)	0.056 (3)	−0.002 (3)	−0.001 (2)	0.004 (3)
C15	0.069 (3)	0.062 (4)	0.067 (3)	0.007 (3)	0.010 (2)	0.004 (3)
C16	0.055 (3)	0.066 (4)	0.065 (3)	−0.001 (3)	−0.002 (2)	0.015 (3)

C17	0.065 (3)	0.069 (4)	0.049 (2)	−0.006 (3)	−0.010 (2)	0.011 (3)
C18	0.056 (2)	0.051 (3)	0.045 (2)	−0.010 (3)	0.0043 (19)	0.003 (2)
C19	0.072 (3)	0.076 (4)	0.047 (2)	0.001 (3)	0.006 (2)	−0.010 (3)

Geometric parameters (Å, °)

Cl—C16	1.746 (5)	C5—H5C	0.9600
O1—C2	1.443 (6)	C6—C11	1.370 (7)
O1—C3	1.298 (7)	C6—C7	1.373 (7)
O2—C3	1.168 (7)	C7—C8	1.372 (6)
O3—C4	1.426 (6)	C7—H7A	0.9300
O3—C6	1.371 (5)	C8—C9	1.361 (8)
O4—C9	1.414 (6)	C8—H8A	0.9300
O4—C12	1.355 (6)	C9—C10	1.363 (8)
N1—C18	1.375 (6)	C10—C11	1.379 (7)
N1—C19	1.285 (6)	C10—H10A	0.9300
N2—C12	1.294 (7)	C11—H11A	0.9300
N2—C13	1.386 (6)	C12—C19	1.420 (6)
C1—C2	1.455 (9)	C13—C14	1.401 (7)
C1—H1B	0.9600	C13—C18	1.407 (6)
C1—H1C	0.9600	C14—C15	1.376 (7)
C1—H1D	0.9600	C14—H14A	0.9300
C2—H2B	0.9700	C15—C16	1.383 (7)
C2—H2C	0.9700	C15—H15A	0.9300
C3—C4	1.528 (8)	C16—C17	1.362 (7)
C4—C5	1.519 (7)	C17—C18	1.398 (6)
C4—H4A	0.9800	C17—H17A	0.9300
C5—H5A	0.9600	C19—H19A	0.9300
C5—H5B	0.9600		
C3—O1—C2	118.8 (5)	C6—C7—H7A	119.2
C6—O3—C4	119.1 (4)	C9—C8—C7	118.3 (5)
C12—O4—C9	119.8 (4)	C9—C8—H8A	120.9
C19—N1—C18	115.6 (4)	C7—C8—H8A	120.9
C12—N2—C13	114.7 (4)	C8—C9—C10	121.3 (5)
C2—C1—H1B	109.5	C8—C9—O4	120.1 (5)
C2—C1—H1C	109.5	C10—C9—O4	118.1 (5)
C2—C1—H1D	109.5	C9—C10—C11	120.2 (5)
H1B—C1—H1C	109.5	C9—C10—H10A	119.9
H1B—C1—H1D	109.5	C11—C10—H10A	119.9
H1C—C1—H1D	109.5	C6—C11—C10	119.2 (5)
O1—C2—C1	106.4 (6)	C6—C11—H11A	120.4
O1—C2—H2B	110.4	C10—C11—H11A	120.4
C1—C2—H2B	110.4	N2—C12—O4	122.8 (4)
O1—C2—H2C	110.4	N2—C12—C19	123.7 (5)
C1—C2—H2C	110.4	O4—C12—C19	113.5 (5)
H2B—C2—H2C	108.6	N2—C13—C14	118.7 (4)
O2—C3—O1	124.0 (6)	N2—C13—C18	121.4 (4)
O2—C3—C4	125.6 (6)	C14—C13—C18	119.9 (4)
O1—C3—C4	110.4 (5)	C15—C14—C13	119.4 (4)

O3—C4—C5	105.1 (5)	C15—C14—H14A	120.3
O3—C4—C3	109.5 (5)	C13—C14—H14A	120.3
C5—C4—C3	111.4 (4)	C14—C15—C16	119.9 (5)
O3—C4—H4A	110.3	C14—C15—H15A	120.1
C5—C4—H4A	110.3	C16—C15—H15A	120.1
C3—C4—H4A	110.3	C17—C16—C15	122.2 (5)
C4—C5—H5A	109.5	C17—C16—Cl	119.2 (4)
C4—C5—H5B	109.5	C15—C16—Cl	118.6 (5)
H5A—C5—H5B	109.5	C16—C17—C18	119.1 (4)
C4—C5—H5C	109.5	C16—C17—H17A	120.4
H5A—C5—H5C	109.5	C18—C17—H17A	120.4
H5B—C5—H5C	109.5	N1—C18—C17	119.2 (4)
C11—C6—O3	125.7 (5)	N1—C18—C13	121.3 (4)
C11—C6—C7	119.5 (5)	C17—C18—C13	119.5 (5)
O3—C6—C7	114.9 (5)	N1—C19—C12	123.3 (5)
C8—C7—C6	121.5 (5)	N1—C19—H19A	118.3
C8—C7—H7A	119.2	C12—C19—H19A	118.3
C3—O1—C2—C1	−157.4 (6)	C13—N2—C12—C19	−1.0 (8)
C2—O1—C3—O2	0.7 (9)	C9—O4—C12—N2	3.3 (9)
C2—O1—C3—C4	179.7 (5)	C9—O4—C12—C19	−176.8 (5)
C6—O3—C4—C5	159.6 (5)	C12—N2—C13—C14	−179.9 (5)
C6—O3—C4—C3	−80.7 (6)	C12—N2—C13—C18	0.4 (7)
O2—C3—C4—O3	10.5 (8)	N2—C13—C14—C15	179.5 (5)
O1—C3—C4—O3	−168.5 (4)	C18—C13—C14—C15	−0.8 (7)
O2—C3—C4—C5	126.3 (7)	C13—C14—C15—C16	0.4 (8)
O1—C3—C4—C5	−52.7 (8)	C14—C15—C16—C17	−0.3 (8)
C4—O3—C6—C11	4.3 (8)	C14—C15—C16—Cl	−179.3 (4)
C4—O3—C6—C7	−177.8 (5)	C15—C16—C17—C18	0.6 (8)
C11—C6—C7—C8	−1.3 (9)	Cl—C16—C17—C18	179.7 (4)
O3—C6—C7—C8	−179.3 (5)	C19—N1—C18—C17	178.8 (5)
C6—C7—C8—C9	0.3 (8)	C19—N1—C18—C13	−0.9 (7)
C7—C8—C9—C10	0.4 (8)	C16—C17—C18—N1	179.3 (5)
C7—C8—C9—O4	172.5 (5)	C16—C17—C18—C13	−1.0 (7)
C12—O4—C9—C8	81.4 (7)	N2—C13—C18—N1	0.5 (7)
C12—O4—C9—C10	−106.3 (6)	C14—C13—C18—N1	−179.2 (5)
C8—C9—C10—C11	−0.1 (9)	N2—C13—C18—C17	−179.2 (5)
O4—C9—C10—C11	−172.4 (6)	C14—C13—C18—C17	1.1 (7)
O3—C6—C11—C10	179.3 (5)	C18—N1—C19—C12	0.4 (8)
C7—C6—C11—C10	1.5 (9)	N2—C12—C19—N1	0.6 (9)
C9—C10—C11—C6	−0.9 (9)	O4—C12—C19—N1	−179.2 (5)
C13—N2—C12—O4	178.9 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19A···N1^{i}	0.93	2.57	3.396 (7)	149

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

Fig. 1

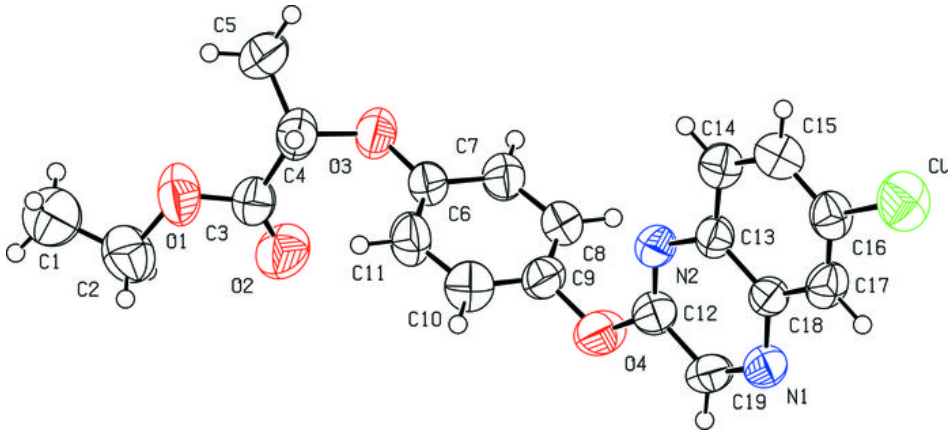
C5
C4
O3
C7
C6
C8
C9
C10
C11
O1
C3
O2
C1
C2
N2
C12
O4
C13
C14
C15
Cl
C16
C17
C18
C19
N1

Fig. 2