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Ethyl 5-(5,6-diphenyl-1,2,4-triazin-3-yl)-2,6-dimethylnicotinate

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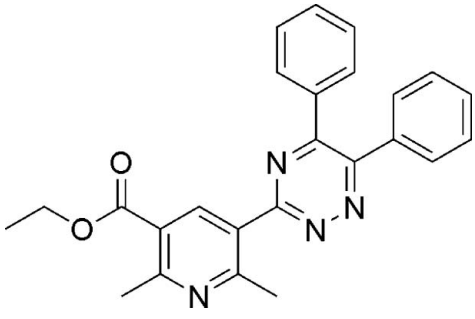
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.207; data-to-parameter ratio = 13.4.

The title nitrogen-donor heterocyclic ligand, $C_{25}H_{22}N_4O_2$, contains a central (1,2,4-triazine) and three attached (two phenyl and a pyridine) rings, all of them having normal bond lengths and angles. The rings are not coplanar, but make dihedral angles with the central triazine ring of 35.96 (6) and 38.49 (8)° (phenyl groups) and 24.92 (3)° (pyridine).

Related literature

For general background, see: Mashaly *et al.* (1999); Zhijian *et al.* (2003); Soudi *et al.* (2005); Eltayeb *et al.* (2006). For related literature, see: Jozsef *et al.* (1988).



Experimental

Crystal data

$C_{25}H_{22}N_4O_2$
M_r = 410.47
Monoclinic, $P2_1/n$
a = 8.9520 (13) Å
b = 27.347 (4) Å
c = 9.2555 (13) Å
β = 107.626 (2)°
V = 2159.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 273 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.97, T_{max} = 0.98
11100 measured reflections
3819 independent reflections
2899 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.208
S = 1.03
3819 reflections
284 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: BG2074).

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supplementary materials

Acta Cryst. (2007). E**63**, o3757 [**doi:10.1107/S1600536807036926**]

Ethyl 5-(5,6-diphenyl-1,2,4-triazin-3-yl)-2,6-dimethylnicotinate

D.-L. Lu, M. Zhang, L.-P. Song, P.-G. Huang and L.-Y. Xu

Comment

1,2,4-Triazines are well known nitrogen-containing heterocyclic compounds which show interesting biological activities and pharmacological properties (Zhijian *et al.*, 2003; Soudi *et al.*, 2005). Some can be active as blood platelet aggregation inhibitors and others exhibit antiviral inhibitory activity, significant activity towards leukemia and ovarian cancer, and anti-HIV activity (Mashaly *et al.*, 1999). Meanwhile, the 3,5,6-trisubstituted 1,2,4-triazines are a principal class of N-donor heterocyclic ligands (Eltayeb *et al.*, 2006). This useful applications for the 1,2,4-triazine derivatives attracted our attention, and here we present a new 3,5,6-trisubstituted 1,2,4-triazine compound, 3-carbethoxy-5-(5,6-diphenyl-1,2,4-triazin-3-yl)-2,6-dimethylpyridine (I).

Fig. 1 shows a molecular diagram of (I). Bond distances in the central 1,2,4-triazine group are in good agreement with those found elsewhere (Jozsef *et al.*, 1988). The rings in the structure are not coplanar, but subtend to the central triazine dihedral angles of 35.96 (6) and 38.49 (8)° (phenyl groups) and 24.92 (3)° (pyridine).

There are no significant H-bonds nor π—π contacts in the structure, the main stabilizing interactions being two very weak intermolecular C—H···π contacts with H···*Cg* distances of C10—H10···*Cg* (N2→ C6)^{i}: 2.93 Å; C18—H18···*Cg* (C9→ C14)^{ii}: 2.95 Å, (i): 2 − *x*, 2 − *y*, 2 − *z*; (ii): −1 + *x*, *y*, *z*.

Experimental

0.01 mol quantities of 3-carboxhydrazide-5-carbethoxy-2, 6-Dimethylpyridine, benzil, and ammonium acetate were disslved in 50 ml of glacial acetic acid. The reaction was refluxed for 4 h, and allowed to cool to room temperature. The reaction mixture was poured into crushed ice, then neutralized with ammonia solution (25%). The solid separated was filtered off, washed with water, dried and recrystallized from ethyl acetate afford pure product in a yield of 68% (m.p. 373 K–374 K). IR (ν, cm^{-1}): 3413 (pyridine CH), 3058 (Ar CH), 1717 (C=O), 1496–1593 (C=C, C=N); ^{1}H-NMR (500 MHz,$CDCl_3$) δ 9.04 (s, 1H, pyridine CH), 7.37–7.68 (m, 10H, Ar CH), 4.41 (q, J=7.0 Hz, 2H, CH), 3.01 (s, 3H, pyridine CH), 2.93 (s, 3H, pyridine CH), 1.42 (t, J=7.0 Hz, 3H, CH); Element analysis, calculate for $C_{25}H_{22}N_4O_2$: C 73.15, H 5.40, N 13.65%; Found: C 73.31, H 5.39, N 13.49%. Single crystals suitable for X-ray analysis were obtained from ethyl acetate by slow evaporation at room temperature.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding model, U_{iso}(H) = 1.2U_{eq}(C).

Figures

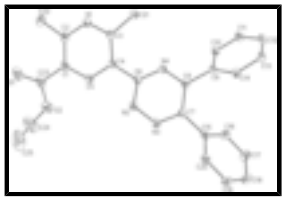


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Fig. 2. The formation of the title compound.

Ethyl 5-(5,6-diphenyl-1,2,4-triazin-3-yl)-2,6-dimethylnicotinate

Crystal data

$C_{25}H_{22}N_4O_2$	F_{000} = 864
M_r = 410.47	D_x = 1.263 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3681 reflections
a = 8.9520 (13) Å	θ = 2.5–27.3º
b = 27.347 (4) Å	μ = 0.08 mm^{-1}
c = 9.2555 (13) Å	T = 273 (2) K
β = 107.626 (2)º	Block, yellow
V = 2159.4 (5) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3819 independent reflections
Radiation source: fine-focus sealed tube	2899 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 273(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→8
T_{min} = 0.97, T_{max} = 0.98	k = −31→32
11100 measured reflections	l = −10→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.064	H-atom parameters constrained
$wR(F^2)$ = 0.208	$w = 1/[\sigma^2(F_o^2) + (0.1109P)^2 + 1.2017P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3819 reflections	$\Delta\rho_{max} = 0.66$ e Å^{-3}
284 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
1 restraint	Extinction correction: ?
Primary atom site location: structure-invariant direct methods	Extinction coefficient: ?

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.1163 (4)	0.84669 (10)	0.5849 (4)	0.0622 (8)
C2	1.2772 (3)	0.85283 (9)	0.6130 (3)	0.0563 (7)
C3	1.2660 (3)	0.93299 (9)	0.6957 (3)	0.0457 (6)
C4	1.1032 (3)	0.92964 (9)	0.6701 (3)	0.0455 (6)
C5	1.0320 (3)	0.88554 (10)	0.6165 (3)	0.0597 (8)
H5	0.9250	0.8819	0.6014	0.072*
C6	1.0030 (3)	0.97025 (9)	0.6923 (3)	0.0450 (6)
C7	0.8047 (3)	1.03660 (9)	0.7319 (3)	0.0434 (6)
C8	0.9678 (3)	1.04098 (8)	0.8068 (3)	0.0421 (6)
C9	1.0435 (3)	1.08365 (8)	0.8995 (3)	0.0442 (6)
C10	1.1687 (3)	1.07663 (10)	1.0289 (3)	0.0528 (7)
H10	1.2022	1.0451	1.0597	0.063*
C11	1.2443 (4)	1.11606 (12)	1.1128 (4)	0.0687 (9)
H11	1.3264	1.1110	1.2012	0.082*
C12	1.1978 (4)	1.16274 (12)	1.0653 (5)	0.0779 (10)
H12	1.2488	1.1894	1.1214	0.093*
C13	1.0758 (4)	1.17022 (11)	0.9348 (5)	0.0758 (10)
H13	1.0463	1.2019	0.9019	0.091*
C14	0.9973 (3)	1.13108 (10)	0.8528 (4)	0.0586 (7)
H14	0.9133	1.1364	0.7661	0.070*
C15	0.6798 (3)	1.06761 (9)	0.7592 (3)	0.0434 (6)
C16	0.6864 (3)	1.08346 (11)	0.9026 (3)	0.0568 (7)
H16	0.7736	1.0760	0.9842	0.068*
C17	0.5656 (4)	1.11024 (12)	0.9265 (4)	0.0685 (9)
H17	0.5712	1.1205	1.0238	0.082*

C18	0.4363 (4)	1.12181 (12)	0.8058 (4)	0.0667 (8)
H18	0.3550	1.1402	0.8213	0.080*
C19	0.4280 (3)	1.10616 (11)	0.6629 (4)	0.0636 (8)
H19	0.3411	1.1141	0.5816	0.076*
C20	0.5471 (3)	1.07877 (10)	0.6384 (3)	0.0527 (7)
H20	0.5391	1.0677	0.5414	0.063*
C21	1.3629 (3)	0.97780 (10)	0.7517 (4)	0.0588 (7)
H21A	1.3818	0.9810	0.8590	0.088*
H21B	1.3078	1.0061	0.7013	0.088*
H21C	1.4611	0.9750	0.7305	0.088*
C22	1.3846 (4)	0.81431 (12)	0.5858 (5)	0.0842 (11)
H22A	1.4891	0.8271	0.6103	0.126*
H22B	1.3498	0.8047	0.4811	0.126*
H22C	1.3836	0.7864	0.6485	0.126*
C23	1.0342 (5)	0.80023 (13)	0.5232 (6)	0.1055 (16)
C24	0.8112 (11)	0.7428 (3)	0.5597 (12)	0.232 (5)
H24A	0.8784	0.7144	0.5688	0.279*
H24B	0.7548	0.7423	0.6342	0.279*
C25	0.7089 (14)	0.7541 (3)	0.3971 (10)	0.226 (4)
H25A	0.6412	0.7812	0.3984	0.239*
H25B	0.6467	0.7259	0.3555	0.239*
H25C	0.7749	0.7621	0.3359	0.239*
N1	1.3472 (3)	0.89480 (8)	0.6680 (3)	0.0533 (6)
N2	0.8542 (3)	0.96875 (8)	0.6040 (3)	0.0604 (7)
N3	0.7536 (3)	1.00124 (8)	0.6299 (3)	0.0588 (6)
N4	1.0635 (2)	1.00556 (7)	0.7928 (2)	0.0453 (5)
O1	1.0835 (4)	0.77057 (12)	0.4538 (6)	0.1622 (19)
O2	0.8981 (4)	0.79630 (11)	0.5471 (6)	0.167 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0636 (18)	0.0408 (15)	0.073 (2)	0.0006 (13)	0.0062 (15)	−0.0113 (13)
C2	0.0665 (18)	0.0415 (14)	0.0588 (17)	0.0069 (13)	0.0156 (14)	−0.0015 (12)
C3	0.0518 (15)	0.0410 (13)	0.0435 (14)	0.0006 (11)	0.0132 (11)	0.0013 (10)
C4	0.0478 (14)	0.0390 (13)	0.0455 (14)	−0.0002 (10)	0.0078 (11)	−0.0029 (10)
C5	0.0500 (15)	0.0463 (15)	0.0738 (19)	−0.0004 (12)	0.0050 (14)	−0.0090 (13)
C6	0.0450 (13)	0.0394 (13)	0.0460 (14)	−0.0016 (10)	0.0068 (11)	−0.0030 (10)
C7	0.0440 (13)	0.0400 (13)	0.0429 (13)	−0.0003 (10)	0.0081 (10)	0.0024 (10)
C8	0.0433 (13)	0.0376 (12)	0.0437 (14)	−0.0007 (10)	0.0109 (10)	0.0025 (10)
C9	0.0426 (13)	0.0394 (13)	0.0524 (15)	−0.0036 (10)	0.0172 (11)	−0.0051 (11)
C10	0.0489 (15)	0.0496 (15)	0.0566 (16)	−0.0051 (12)	0.0110 (12)	−0.0062 (12)
C11	0.0586 (18)	0.073 (2)	0.070 (2)	−0.0156 (15)	0.0137 (15)	−0.0237 (16)
C12	0.072 (2)	0.058 (2)	0.106 (3)	−0.0209 (16)	0.030 (2)	−0.0367 (19)
C13	0.072 (2)	0.0389 (15)	0.119 (3)	−0.0041 (14)	0.033 (2)	−0.0110 (17)
C14	0.0559 (17)	0.0409 (14)	0.077 (2)	−0.0001 (12)	0.0176 (14)	0.0000 (13)
C15	0.0402 (13)	0.0411 (13)	0.0481 (14)	−0.0033 (10)	0.0121 (11)	0.0039 (10)
C16	0.0535 (16)	0.0703 (18)	0.0458 (15)	0.0084 (13)	0.0138 (12)	0.0053 (13)

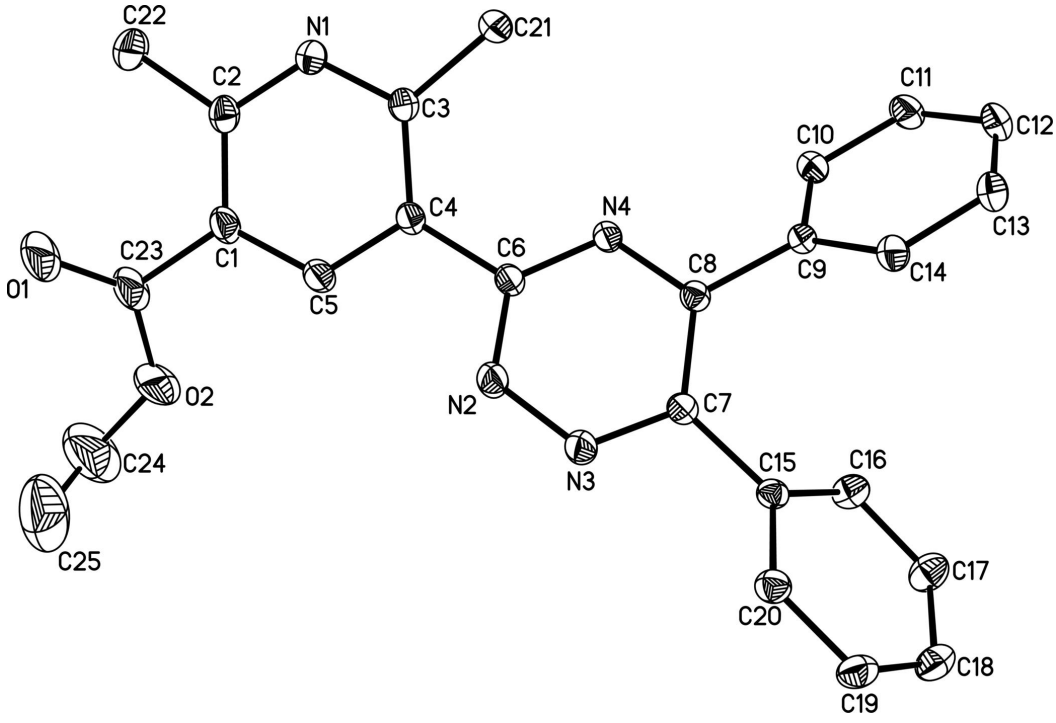
C17	0.069 (2)	0.084 (2)	0.0581 (18)	0.0143 (16)	0.0267 (16)	0.0016 (16)
C18	0.0558 (18)	0.071 (2)	0.080 (2)	0.0131 (15)	0.0306 (16)	0.0060 (16)
C19	0.0451 (15)	0.0709 (19)	0.070 (2)	0.0093 (14)	0.0094 (14)	0.0069 (15)
C20	0.0475 (15)	0.0558 (16)	0.0511 (15)	−0.0001 (12)	0.0096 (12)	0.0001 (12)
C21	0.0529 (16)	0.0486 (15)	0.0764 (19)	−0.0070 (12)	0.0220 (14)	−0.0073 (14)
C22	0.085 (2)	0.0569 (19)	0.116 (3)	0.0132 (17)	0.038 (2)	−0.0128 (19)
C23	0.084 (3)	0.049 (2)	0.158 (4)	0.0046 (19)	−0.001 (3)	−0.039 (2)
C24	0.106 (8)	0.109 (5)	0.133 (14)	−0.017 (5)	−0.010 (8)	−0.064 (7)
C25	0.128 (13)	0.102 (6)	0.126 (10)	0.022 (7)	0.047 (9)	−0.051 (6)
N1	0.0554 (13)	0.0464 (12)	0.0588 (14)	0.0037 (10)	0.0181 (11)	−0.0023 (10)
N2	0.0529 (13)	0.0544 (13)	0.0614 (15)	0.0071 (11)	−0.0012 (11)	−0.0152 (11)
N3	0.0496 (13)	0.0539 (13)	0.0628 (15)	0.0059 (10)	0.0017 (11)	−0.0124 (11)
N4	0.0437 (11)	0.0388 (11)	0.0501 (12)	−0.0009 (9)	0.0094 (9)	−0.0046 (9)
O1	0.115 (3)	0.086 (2)	0.262 (5)	0.0002 (18)	0.021 (3)	−0.099 (3)
O2	0.098 (2)	0.081 (2)	0.116 (6)	−0.0437 (18)	0.052 (3)	−0.086 (3)

Geometric parameters (Å, °)

C1—C5	1.385 (4)	C14—H14	0.9300
C1—C2	1.394 (4)	C15—C16	1.380 (4)
C1—C23	1.492 (4)	C15—C20	1.397 (4)
C2—N1	1.332 (3)	C16—C17	1.378 (4)
C2—C22	1.498 (4)	C16—H16	0.9300
C3—N1	1.341 (3)	C17—C18	1.381 (4)
C3—C4	1.407 (4)	C17—H17	0.9300
C3—C21	1.500 (4)	C18—C19	1.370 (5)
C4—C5	1.384 (4)	C18—H18	0.9300
C4—C6	1.481 (3)	C19—C20	1.376 (4)
C5—H5	0.9300	C19—H19	0.9300
C6—N4	1.336 (3)	C20—H20	0.9300
C6—N2	1.335 (3)	C21—H21A	0.9600
C7—N3	1.331 (3)	C21—H21B	0.9600
C7—C8	1.419 (3)	C21—H21C	0.9600
C7—C15	1.485 (3)	C22—H22A	0.9600
C8—N4	1.325 (3)	C22—H22B	0.9600
C8—C9	1.485 (3)	C22—H22C	0.9600
C9—C10	1.384 (4)	C23—O1	1.199 (5)
C9—C14	1.390 (4)	C23—O2	1.307 (6)
C10—C11	1.380 (4)	C24—C25	1.538 (11)
C10—H10	0.9300	C24—O2	1.678 (9)
C11—C12	1.373 (5)	C24—H24A	0.9700
C11—H11	0.9300	C24—H24B	0.9700
C12—C13	1.376 (5)	C25—H25A	0.9600
C12—H12	0.9300	C25—H25B	0.9600
C13—C14	1.375 (4)	C25—H25C	0.9600
C13—H13	0.9300	N2—N3	1.338 (3)
C5—C1—C2	117.8 (3)	C17—C16—H16	119.5
C5—C1—C23	119.8 (3)	C15—C16—H16	119.5
C2—C1—C23	122.4 (3)	C16—C17—C18	119.9 (3)

N1—C2—C1	121.0 (2)	C16—C17—H17	120.1
N1—C2—C22	114.7 (3)	C18—C17—H17	120.1
C1—C2—C22	124.3 (3)	C19—C18—C17	119.8 (3)
N1—C3—C4	120.7 (2)	C19—C18—H18	120.1
N1—C3—C21	114.3 (2)	C17—C18—H18	120.1
C4—C3—C21	124.9 (2)	C18—C19—C20	120.7 (3)
C5—C4—C3	117.3 (2)	C18—C19—H19	119.7
C5—C4—C6	118.0 (2)	C20—C19—H19	119.7
C3—C4—C6	124.6 (2)	C19—C20—C15	120.0 (3)
C4—C5—C1	121.5 (3)	C19—C20—H20	120.0
C4—C5—H5	119.3	C15—C20—H20	120.0
C1—C5—H5	119.3	C3—C21—H21A	109.5
N4—C6—N2	124.5 (2)	C3—C21—H21B	109.5
N4—C6—C4	120.2 (2)	H21A—C21—H21B	109.5
N2—C6—C4	115.2 (2)	C3—C21—H21C	109.5
N3—C7—C8	119.3 (2)	H21A—C21—H21C	109.5
N3—C7—C15	114.9 (2)	H21B—C21—H21C	109.5
C8—C7—C15	125.8 (2)	C2—C22—H22A	109.5
N4—C8—C7	119.4 (2)	C2—C22—H22B	109.5
N4—C8—C9	115.8 (2)	H22A—C22—H22B	109.5
C7—C8—C9	124.8 (2)	C2—C22—H22C	109.5
C10—C9—C14	119.0 (2)	H22A—C22—H22C	109.5
C10—C9—C8	120.0 (2)	H22B—C22—H22C	109.5
C14—C9—C8	120.9 (2)	O1—C23—O2	123.2 (4)
C11—C10—C9	120.6 (3)	O1—C23—C1	124.2 (5)
C11—C10—H10	119.7	O2—C23—C1	112.5 (3)
C9—C10—H10	119.7	C25—C24—O2	84.7 (6)
C12—C11—C10	119.8 (3)	C25—C24—H24A	114.5
C12—C11—H11	120.1	O2—C24—H24A	114.5
C10—C11—H11	120.1	C25—C24—H24B	114.5
C11—C12—C13	120.1 (3)	O2—C24—H24B	114.5
C11—C12—H12	119.9	H24A—C24—H24B	111.6
C13—C12—H12	119.9	C24—C25—H25A	109.5
C12—C13—C14	120.4 (3)	C24—C25—H25B	109.5
C12—C13—H13	119.8	H25A—C25—H25B	109.5
C14—C13—H13	119.8	C24—C25—H25C	109.5
C13—C14—C9	120.0 (3)	H25A—C25—H25C	109.5
C13—C14—H14	120.0	H25B—C25—H25C	109.5
C9—C14—H14	120.0	C2—N1—C3	121.6 (2)
C16—C15—C20	118.7 (2)	C6—N2—N3	118.1 (2)
C16—C15—C7	121.9 (2)	C7—N3—N2	120.3 (2)
C20—C15—C7	119.4 (2)	C8—N4—C6	117.3 (2)
C17—C16—C15	120.9 (3)	C23—O2—C24	124.0 (4)

Fig. 1


C22
N1
C21
C2
C3
C11
C12
C10
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N4
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C23
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C9
C14
O1
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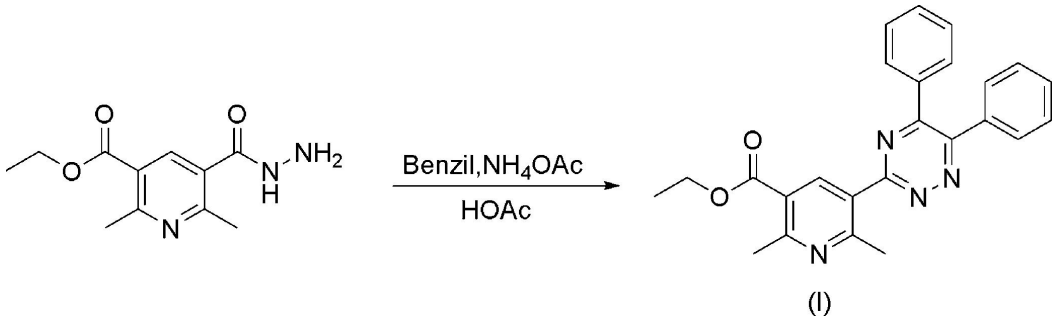
C18
C19

Fig. 2



(I)