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3,5-Bis[4-(dimethylamino)benzylidene]-1-propyl-4-piperidone: a prospective biophotonic material

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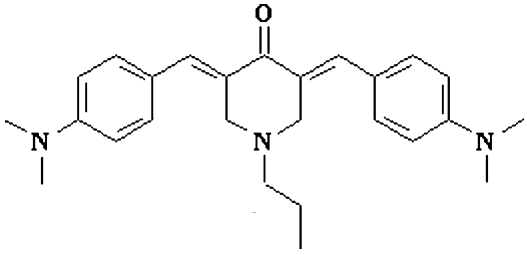
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.134; data-to-parameter ratio = 15.6.

In the title compound, $C_{26}H_{33}N_3O$, the central heterocyclic ring exhibits a flattened boat conformation, with the N and the opposite C atom displaced from the plane of the other four C atoms. The dihedral angles between the planar part of the heterocycle and the two almost flat fragments which include the benzene rings and attached C atoms are 17.1 (1) and 14.8 (1)°. This conformation helps promote conjugation in the molecule. Bond-length distributions in the π-conjugated bridges and *p*-dimethylaminophenyl fragments show an alternation of single C—C and double C=C bond lengths. In the crystal structure, weak C—H···O hydrogen bonds link the molecules into ribbons along the *b* axis.

Related literature

For related literature, see: Desiraju & Steiner (1999); Dimmock *et al.* (2001); Jia *et al.* (1989); Nesterov (2004); Nesterov *et al.* (2003, 2007); Sarkisov *et al.* (2005).



Experimental

Crystal data

$C_{26}H_{33}N_3O$
M_r = 403.55
Monoclinic, $P2_1/n$
a = 14.7200 (9) Å
b = 6.1434 (4) Å
c = 24.2503 (16) Å
β = 92.262 (1)°
V = 2191.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 (2) K
0.12 × 0.04 × 0.04 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.912, T_{max} = 0.997
18187 measured reflections
4296 independent reflections
2976 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.134
S = 1.01
4296 reflections
276 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.242 (2)	C5—C14	1.351 (3)
N2—C11	1.365 (3)	C7—C8	1.453 (3)
N3—C18	1.374 (3)	C14—C15	1.449 (3)
C3—C7	1.346 (3)		
C4—C3—C7—C8	−175.9 (2)	C4—C5—C14—C15	177.6 (2)
C3—C7—C8—C9	−168.4 (2)	C5—C14—C15—C16	164.8 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O1^{i}	0.95	2.56	3.371 (3)	143
C22—H22C···O1^{ii}	0.98	2.48	3.364 (3)	150

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL-NT* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2143).

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supplementary materials

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3,5-Bis[4-(dimethylamino)benzylidene]-1-propyl-4-piperidone: a prospective biophotonic material

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Comment

As a continuation of our work that includes synthesis and structural investigations of nonlinear optical organic compounds with two-photon absorption properties and potential as biophotonic materials (Nesterov *et al.*, 2003; Nesterov, 2004; Sarkisov *et al.*, 2005; Nesterov *et al.*, 2007), we have investigated the structure of the title compound that has a general motif D-π-A-π-D (Scheme). This compound may find application as an agent for locating cancer cells with two-photon excited fluorescence and as a potential agent for a photodynamic treatment of cancer (Nesterov *et al.*, 2003; Sarkisov *et al.*, 2005).

The title compound belongs to a group that has shown anticancer activity (Dimmock *et al.*, 2001) and here we describe its structure (Fig. 1). The central heterocycle adopts a flattened boat conformation; atoms N1 and C4 lie 0.699 (2) and 0.118 (2) Å, respectively, out of the C2/C3/C5/C6 plane [planar within 0.023 (2) Å]. Dihedral angles between the planar part of the heterocycle and two almost flat fragments that include the benzene rings and attached C atoms are 17.1 (1) and 14.8 (1)° for C7—C13 and C14—C20, respectively. This might be partly due to the presence in the molecule of short intramolecular contacts H2B···H13A and H6A···H20A with distances 2.06 and 2.18 Å, respectively, that are somewhat shorter than the sum of the van der Waals radii (2.2 Å) of the hydrogen atoms (Rowland & Taylor, 1996).

Atom N1 in the piperidone ring is pyramidal, with the sum of bond angles equal to 328.0°; the propyl substituent attached to it occupies the equatorial position. Bond length distributions in the π-conjugated bridges and *p*-dimethylaminophenyl fragments definitely show an alternation of single C—C and double C═C bond lengths (Table) and close to the standard conjugated values (Allen *et al.*, 1987). In the crystal structure, there are weak intermolecular C—H···O contacts that can be considered as weak hydrogen bonds (Desiraju & Steiner, 1999). Such weak hydrogen bonds link the molecules into ribbons along the *b* axis (Fig. 2).

Experimental

The title compound was obtained according to literature procedures (Jia *et al.*, 1989; Nesterov *et al.*, 2003) by the reaction of *p*-dimethylaminobenzaldehyde with 1-propyl-4-piperidone. The precipitate was isolated and recrystallized from ethanol/tetrahydrofuran (1:1) (melting point 464 K, yield 76%). Crystals were obtained by isothermic evaporation of an ethanolic solution. The structure of the compound was characterized by ^{1}H and ^{13}C NMR spectroscopy.

Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H distances of 0.95 Å for Csp^2, with U_{iso}(H) = 1.2U_{eq}(C); 0.99 Å for CH_2, with U_{iso} (H) = 1.2U_{eq}(C); 0.98 Å for CH_3, with U_{iso}(H) = 1.5U_{eq}(C).

Figures

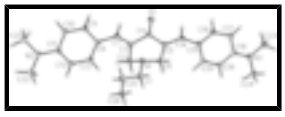

Fig. 1. The moleculatr structure of the title compound, with the atom-numbering scheme. The non-H atoms are shown with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as circles of arbitrary small radius.

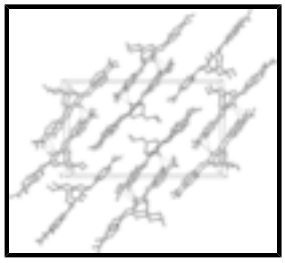

Fig. 2. Projection of the crystal packing along the *b* axis. Dashed lines denote intermolecular C—H···O hydrogen bonds. Only H atoms participating in hydrogen bonds are shown.

3,5-Bis(4-dimethylaminobenzylidene)-1-propyl-4-piperidone

Crystal data

$C_{26}H_{33}N_3O$	F_{000} = 872
M_r = 403.55	D_x = 1.223 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.7200 (9) Å	Cell parameters from 117 reflections
b = 6.1434 (4) Å	θ = 4–24º
c = 24.2503 (16) Å	μ = 0.08 mm^{-1}
β = 92.262 (1)º	T = 100 (2) K
V = 2191.3 (2) Å^3	Needle, yellow
Z = 4	0.12 × 0.04 × 0.04 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	4296 independent reflections
Radiation source: fine-focus sealed tube	2976 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
T = 100(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −18→18
T_{min} = 0.912, T_{max} = 0.997	k = −7→7
18187 measured reflections	l = −29→29

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

$wR(F^2) = 0.134$	$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 1.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
4296 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
276 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
O1	0.24493 (10)	0.9379 (2)	0.58185 (6)	0.0272 (4)
N1	0.36050 (11)	0.4318 (3)	0.50843 (7)	0.0226 (4)
N2	−0.13269 (12)	0.4966 (3)	0.34015 (7)	0.0271 (4)
N3	0.66819 (13)	0.5195 (3)	0.79613 (7)	0.0294 (4)
C1	0.40071 (15)	0.2306 (4)	0.48621 (9)	0.0292 (5)
H1A	0.3783	0.1047	0.5073	0.035*
H1B	0.4675	0.2372	0.4925	0.035*
C2	0.26123 (13)	0.4304 (3)	0.50017 (9)	0.0230 (5)
H2A	0.2355	0.3067	0.5205	0.028*
H2B	0.2450	0.4110	0.4605	0.028*
C3	0.22117 (13)	0.6403 (3)	0.52019 (8)	0.0201 (4)
C4	0.26981 (14)	0.7562 (3)	0.56591 (8)	0.0215 (5)
C5	0.34805 (13)	0.6429 (3)	0.59400 (8)	0.0205 (4)
C6	0.38466 (14)	0.4402 (3)	0.56754 (8)	0.0225 (5)
H6A	0.4517	0.4370	0.5729	0.027*
H6B	0.3598	0.3102	0.5858	0.027*
C7	0.14321 (13)	0.7289 (3)	0.49991 (8)	0.0206 (4)
H7A	0.1292	0.8655	0.5159	0.025*
C8	0.07633 (13)	0.6557 (3)	0.45827 (8)	0.0201 (4)
C9	0.01067 (14)	0.8070 (3)	0.43939 (8)	0.0239 (5)
H9A	0.0135	0.9506	0.4539	0.029*
C10	−0.05739 (14)	0.7584 (3)	0.40107 (9)	0.0242 (5)
H10A	−0.1000	0.8676	0.3900	0.029*
C11	−0.06472 (14)	0.5473 (3)	0.37789 (8)	0.0216 (4)
C12	0.00081 (13)	0.3930 (3)	0.39659 (8)	0.0214 (5)

H12A	−0.0014	0.2498	0.3818	0.026*
C13	0.06775 (13)	0.4452 (3)	0.43573 (8)	0.0209 (4)
H13A	0.1094	0.3356	0.4479	0.025*
C14	0.37999 (13)	0.7282 (3)	0.64231 (9)	0.0226 (5)
H14A	0.3499	0.8577	0.6527	0.027*
C15	0.45150 (13)	0.6596 (3)	0.68130 (8)	0.0214 (4)
C16	0.48335 (14)	0.8106 (3)	0.72105 (9)	0.0255 (5)
H16A	0.4554	0.9499	0.7218	0.031*
C17	0.55279 (15)	0.7671 (3)	0.75880 (9)	0.0266 (5)
H17A	0.5720	0.8763	0.7844	0.032*
C18	0.59610 (14)	0.5619 (3)	0.76001 (8)	0.0234 (5)
C19	0.56228 (14)	0.4060 (3)	0.72189 (8)	0.0235 (5)
H19A	0.5880	0.2641	0.7223	0.028*
C20	0.49298 (14)	0.4537 (3)	0.68410 (8)	0.0239 (5)
H20A	0.4725	0.3437	0.6590	0.029*
C21	−0.19772 (15)	0.6606 (4)	0.32053 (9)	0.0290 (5)
H21A	−0.2211	0.7395	0.3521	0.044*
H21B	−0.2482	0.5895	0.3001	0.044*
H21C	−0.1676	0.7629	0.2962	0.044*
C22	−0.13508 (15)	0.2850 (3)	0.31302 (9)	0.0274 (5)
H22A	−0.0746	0.2506	0.2999	0.041*
H22B	−0.1791	0.2887	0.2817	0.041*
H22C	−0.1531	0.1733	0.3393	0.041*
C23	0.69416 (16)	0.6790 (4)	0.83827 (10)	0.0354 (6)
H23A	0.7150	0.8123	0.8206	0.053*
H23B	0.7433	0.6197	0.8622	0.053*
H23C	0.6416	0.7123	0.8604	0.053*
C24	0.70289 (16)	0.3012 (4)	0.80339 (9)	0.0304 (5)
H24A	0.7107	0.2344	0.7672	0.046*
H24B	0.6599	0.2148	0.8241	0.046*
H24D	0.7616	0.3063	0.8238	0.046*
C25	0.38018 (16)	0.1914 (4)	0.42620 (9)	0.0323 (6)
H25A	0.4025	0.3158	0.4046	0.039*
H25C	0.3136	0.1808	0.4194	0.039*
C26	0.42548 (16)	−0.0191 (4)	0.40712 (10)	0.0335 (6)
H26D	0.4099	−0.0436	0.3680	0.050*
H26A	0.4039	−0.1420	0.4288	0.050*
H26B	0.4916	−0.0062	0.4124	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0317 (8)	0.0175 (7)	0.0320 (8)	0.0061 (6)	−0.0055 (7)	−0.0053 (6)
N1	0.0213 (9)	0.0218 (9)	0.0244 (9)	0.0036 (7)	−0.0033 (7)	−0.0061 (7)
N2	0.0326 (10)	0.0173 (9)	0.0303 (10)	0.0027 (8)	−0.0105 (8)	−0.0004 (8)
N3	0.0348 (11)	0.0213 (10)	0.0311 (10)	0.0020 (8)	−0.0116 (8)	−0.0021 (8)
C1	0.0250 (11)	0.0277 (12)	0.0348 (13)	0.0076 (10)	−0.0027 (10)	−0.0095 (10)
C2	0.0243 (11)	0.0174 (10)	0.0271 (11)	0.0020 (9)	−0.0021 (9)	−0.0061 (9)

C3	0.0226 (10)	0.0156 (10)	0.0220 (11)	0.0004 (8)	0.0022 (8)	0.0008 (8)
C4	0.0254 (11)	0.0145 (10)	0.0249 (11)	0.0009 (9)	0.0035 (9)	−0.0017 (8)
C5	0.0201 (10)	0.0167 (10)	0.0248 (11)	0.0003 (8)	0.0007 (8)	−0.0004 (8)
C6	0.0224 (11)	0.0178 (10)	0.0271 (11)	0.0046 (8)	−0.0036 (9)	−0.0025 (9)
C7	0.0252 (11)	0.0157 (10)	0.0211 (10)	0.0020 (8)	0.0017 (8)	0.0007 (8)
C8	0.0210 (10)	0.0178 (10)	0.0216 (11)	0.0004 (8)	0.0014 (8)	0.0017 (8)
C9	0.0298 (12)	0.0176 (10)	0.0241 (11)	0.0039 (9)	−0.0009 (9)	−0.0015 (9)
C10	0.0275 (11)	0.0176 (10)	0.0271 (12)	0.0060 (9)	−0.0034 (9)	0.0021 (9)
C11	0.0261 (11)	0.0181 (10)	0.0203 (10)	−0.0007 (8)	−0.0007 (9)	0.0021 (8)
C12	0.0256 (11)	0.0141 (10)	0.0244 (11)	0.0004 (8)	0.0004 (9)	0.0002 (8)
C13	0.0219 (10)	0.0151 (10)	0.0256 (11)	0.0043 (8)	0.0007 (8)	0.0033 (8)
C14	0.0228 (11)	0.0165 (10)	0.0284 (12)	0.0027 (8)	0.0021 (9)	−0.0029 (9)
C15	0.0221 (11)	0.0199 (10)	0.0221 (11)	0.0012 (8)	−0.0005 (8)	−0.0020 (9)
C16	0.0287 (11)	0.0185 (11)	0.0290 (12)	0.0040 (9)	−0.0019 (9)	−0.0064 (9)
C17	0.0311 (12)	0.0221 (11)	0.0262 (12)	0.0005 (9)	−0.0030 (9)	−0.0078 (9)
C18	0.0251 (11)	0.0228 (11)	0.0221 (11)	0.0009 (9)	−0.0004 (9)	0.0014 (9)
C19	0.0289 (11)	0.0157 (10)	0.0257 (11)	0.0024 (9)	−0.0015 (9)	−0.0012 (9)
C20	0.0304 (12)	0.0174 (10)	0.0236 (11)	−0.0001 (9)	−0.0012 (9)	−0.0046 (9)
C21	0.0317 (12)	0.0239 (11)	0.0306 (12)	0.0040 (10)	−0.0100 (10)	0.0015 (10)
C22	0.0327 (12)	0.0203 (11)	0.0287 (12)	−0.0001 (9)	−0.0055 (9)	−0.0031 (9)
C23	0.0370 (13)	0.0356 (14)	0.0324 (13)	0.0049 (11)	−0.0124 (11)	−0.0076 (11)
C24	0.0329 (13)	0.0285 (12)	0.0292 (12)	0.0070 (10)	−0.0074 (10)	−0.0004 (10)
C25	0.0316 (12)	0.0320 (13)	0.0331 (13)	0.0069 (10)	−0.0015 (10)	−0.0062 (10)
C26	0.0306 (12)	0.0339 (13)	0.0356 (13)	0.0070 (10)	−0.0029 (10)	−0.0150 (11)

Geometric parameters (Å, °)

O1—C4	1.242 (2)	C12—H12A	0.9500
N1—C6	1.464 (3)	C13—H13A	0.9500
N1—C2	1.467 (3)	C14—C15	1.449 (3)
N1—C1	1.481 (3)	C14—H14A	0.9500
N2—C11	1.365 (3)	C15—C16	1.405 (3)
N2—C21	1.456 (3)	C15—C20	1.405 (3)
N2—C22	1.457 (3)	C16—C17	1.371 (3)
N3—C18	1.374 (3)	C16—H16A	0.9500
N3—C24	1.443 (3)	C17—C18	1.412 (3)
N3—C23	1.456 (3)	C17—H17A	0.9500
C1—C25	1.494 (3)	C18—C19	1.409 (3)
C1—H1A	0.9900	C19—C20	1.376 (3)
C1—H1B	0.9900	C19—H19A	0.9500
C2—C3	1.506 (3)	C20—H20A	0.9500
C2—H2A	0.9900	C21—H21A	0.9800
C2—H2B	0.9900	C21—H21B	0.9800
C3—C7	1.346 (3)	C21—H21C	0.9800
C3—C4	1.478 (3)	C22—H22A	0.9800
C4—C5	1.487 (3)	C22—H22B	0.9800
C5—C14	1.351 (3)	C22—H22C	0.9800
C5—C6	1.510 (3)	C23—H23A	0.9800
C6—H6A	0.9900	C23—H23B	0.9800

C6—H6B	0.9900	C23—H23C	0.9800
C7—C8	1.453 (3)	C24—H24A	0.9800
C7—H7A	0.9500	C24—H24B	0.9800
C8—C9	1.405 (3)	C24—H24D	0.9800
C8—C13	1.408 (3)	C25—C26	1.535 (3)
C9—C10	1.372 (3)	C25—H25A	0.9900
C9—H9A	0.9500	C25—H25C	0.9900
C10—C11	1.416 (3)	C26—H26D	0.9800
C10—H10A	0.9500	C26—H26A	0.9800
C11—C12	1.414 (3)	C26—H26B	0.9800
C12—C13	1.379 (3)		
C6—N1—C2	109.64 (16)	C5—C14—C15	132.23 (19)
C6—N1—C1	107.48 (16)	C5—C14—H14A	113.9
C2—N1—C1	110.84 (16)	C15—C14—H14A	113.9
C11—N2—C21	121.08 (17)	C16—C15—C20	115.38 (18)
C11—N2—C22	120.68 (17)	C16—C15—C14	118.03 (18)
C21—N2—C22	117.76 (17)	C20—C15—C14	126.60 (19)
C18—N3—C24	121.00 (18)	C17—C16—C15	123.31 (19)
C18—N3—C23	119.62 (18)	C17—C16—H16A	118.3
C24—N3—C23	117.24 (17)	C15—C16—H16A	118.3
N1—C1—C25	114.85 (18)	C16—C17—C18	120.78 (19)
N1—C1—H1A	108.6	C16—C17—H17A	119.6
C25—C1—H1A	108.6	C18—C17—H17A	119.6
N1—C1—H1B	108.6	N3—C18—C19	122.22 (19)
C25—C1—H1B	108.6	N3—C18—C17	121.29 (19)
H1A—C1—H1B	107.5	C19—C18—C17	116.48 (18)
N1—C2—C3	110.58 (16)	C20—C19—C18	121.71 (19)
N1—C2—H2A	109.5	C20—C19—H19A	119.1
C3—C2—H2A	109.5	C18—C19—H19A	119.1
N1—C2—H2B	109.5	C19—C20—C15	122.25 (19)
C3—C2—H2B	109.5	C19—C20—H20A	118.9
H2A—C2—H2B	108.1	C15—C20—H20A	118.9
C7—C3—C4	117.38 (18)	N2—C21—H21A	109.5
C7—C3—C2	124.58 (18)	N2—C21—H21B	109.5
C4—C3—C2	118.03 (17)	H21A—C21—H21B	109.5
O1—C4—C3	121.77 (18)	N2—C21—H21C	109.5
O1—C4—C5	120.70 (18)	H21A—C21—H21C	109.5
C3—C4—C5	117.48 (17)	H21B—C21—H21C	109.5
C14—C5—C4	116.91 (18)	N2—C22—H22A	109.5
C14—C5—C6	124.78 (18)	N2—C22—H22B	109.5
C4—C5—C6	118.29 (17)	H22A—C22—H22B	109.5
N1—C6—C5	111.59 (16)	N2—C22—H22C	109.5
N1—C6—H6A	109.3	H22A—C22—H22C	109.5
C5—C6—H6A	109.3	H22B—C22—H22C	109.5
N1—C6—H6B	109.3	N3—C23—H23A	109.5
C5—C6—H6B	109.3	N3—C23—H23B	109.5
H6A—C6—H6B	108.0	H23A—C23—H23B	109.5
C3—C7—C8	132.31 (19)	N3—C23—H23C	109.5
C3—C7—H7A	113.8	H23A—C23—H23C	109.5

C8—C7—H7A	113.8	H23B—C23—H23C	109.5
C9—C8—C13	115.55 (18)	N3—C24—H24A	109.5
C9—C8—C7	117.40 (18)	N3—C24—H24B	109.5
C13—C8—C7	127.00 (18)	H24A—C24—H24B	109.5
C10—C9—C8	123.47 (19)	N3—C24—H24D	109.5
C10—C9—H9A	118.3	H24A—C24—H24D	109.5
C8—C9—H9A	118.3	H24B—C24—H24D	109.5
C9—C10—C11	120.68 (19)	C1—C25—C26	110.83 (19)
C9—C10—H10A	119.7	C1—C25—H25A	109.5
C11—C10—H10A	119.7	C26—C25—H25A	109.5
N2—C11—C12	122.34 (18)	C1—C25—H25C	109.5
N2—C11—C10	121.15 (18)	C26—C25—H25C	109.5
C12—C11—C10	116.50 (18)	H25A—C25—H25C	108.1
C13—C12—C11	121.67 (18)	C25—C26—H26D	109.5
C13—C12—H12A	119.2	C25—C26—H26A	109.5
C11—C12—H12A	119.2	H26D—C26—H26A	109.5
C12—C13—C8	122.10 (18)	C25—C26—H26B	109.5
C12—C13—H13A	118.9	H26D—C26—H26B	109.5
C8—C13—H13A	118.9	H26A—C26—H26B	109.5
C6—N1—C1—C25	178.10 (19)	C22—N2—C11—C10	174.65 (19)
C2—N1—C1—C25	58.3 (2)	C9—C10—C11—N2	179.3 (2)
C6—N1—C2—C3	64.4 (2)	C9—C10—C11—C12	0.3 (3)
C1—N1—C2—C3	−177.10 (17)	N2—C11—C12—C13	−178.40 (19)
N1—C2—C3—C7	151.68 (19)	C10—C11—C12—C13	0.6 (3)
N1—C2—C3—C4	−29.3 (2)	C11—C12—C13—C8	−1.7 (3)
C7—C3—C4—O1	−6.5 (3)	C9—C8—C13—C12	1.7 (3)
C2—C3—C4—O1	174.41 (19)	C7—C8—C13—C12	179.35 (19)
C7—C3—C4—C5	171.03 (18)	C4—C5—C14—C15	177.6 (2)
C2—C3—C4—C5	−8.1 (3)	C6—C5—C14—C15	−1.0 (4)
O1—C4—C5—C14	10.8 (3)	C5—C14—C15—C16	164.8 (2)
C3—C4—C5—C14	−166.72 (18)	C5—C14—C15—C20	−15.8 (4)
O1—C4—C5—C6	−170.44 (19)	C20—C15—C16—C17	2.8 (3)
C3—C4—C5—C6	12.0 (3)	C14—C15—C16—C17	−177.7 (2)
C2—N1—C6—C5	−60.5 (2)	C15—C16—C17—C18	−0.8 (3)
C1—N1—C6—C5	178.94 (17)	C24—N3—C18—C19	−10.8 (3)
C14—C5—C6—N1	−159.57 (19)	C23—N3—C18—C19	−173.8 (2)
C4—C5—C6—N1	21.8 (3)	C24—N3—C18—C17	170.1 (2)
C4—C3—C7—C8	−175.9 (2)	C23—N3—C18—C17	7.1 (3)
C2—C3—C7—C8	3.1 (4)	C16—C17—C18—N3	177.3 (2)
C3—C7—C8—C9	−168.4 (2)	C16—C17—C18—C19	−1.8 (3)
C3—C7—C8—C13	14.0 (4)	N3—C18—C19—C20	−176.8 (2)
C13—C8—C9—C10	−0.8 (3)	C17—C18—C19—C20	2.4 (3)
C7—C8—C9—C10	−178.65 (19)	C18—C19—C20—C15	−0.3 (3)
C8—C9—C10—C11	−0.2 (3)	C16—C15—C20—C19	−2.3 (3)
C21—N2—C11—C12	−178.29 (19)	C14—C15—C20—C19	178.3 (2)
C22—N2—C11—C12	−6.4 (3)	N1—C1—C25—C26	179.46 (19)
C21—N2—C11—C10	2.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10A···O1^{i}	0.95	2.56	3.371 (3)	143
C22—H22C···O1^{ii}	0.98	2.48	3.364 (3)	150

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

Fig. 1

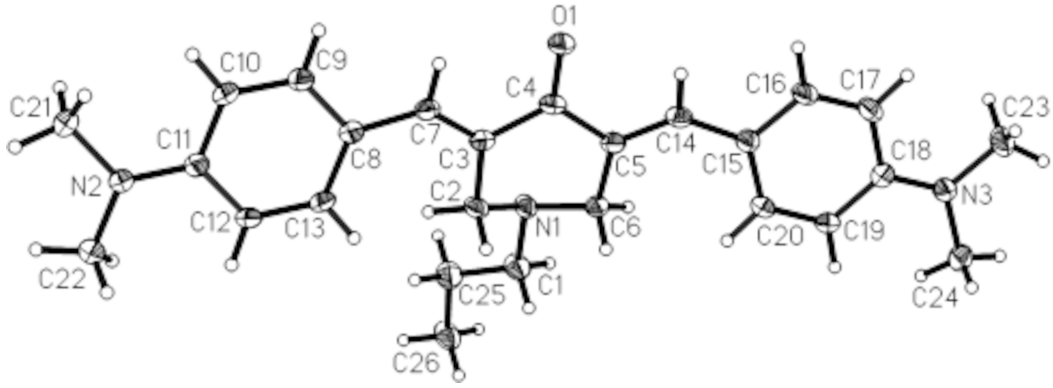
O1
C10
C9
C4
C16
C17
C21
C23
C11
C7
C3
C5
C14
C15
C18
C8
N2
C2
N3
C12
C13
N1
C6
C20
C19
C22
C25
C1
C24
C26

Fig. 2