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3-[(2-Hydroxy-1-naphthyl)(piperidin-1-yl)methyl]benzonitrile

Zhi-Rong Qu

Ordered Matter Science Research Center, School of Chemistry and Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China
Correspondence e-mail: xraylab@hotmail.com

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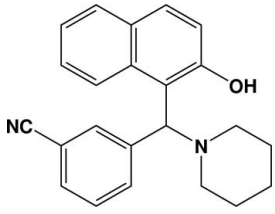
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.100; data-to-parameter ratio = 15.7.

Molecules of the title compound, $C_{23}H_{22}N_2O$, have normal geometric parameters. An intramolecular O—H···N hydrogen bond stabilizes the molecular conformation. The crystal packing is characterized by helical chains of molecules linked by C—H···O hydrogen bonds.

Related literature

For unnatural homochiral aminophenol compounds obtained by Betti-type reaction, see: Lu *et al.* (2002); Xu *et al.* (2004); Wang *et al.* (2005).



Experimental

Crystal data

$C_{23}H_{22}N_2O$
M_r = 342.43
Monoclinic, $P2_1/c$
a = 11.9008 (13) Å
b = 15.0138 (17) Å
c = 10.8886 (13) Å
β = 102.867 (3)°
V = 1896.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.98, T_{max} = 0.98
11353 measured reflections
3731 independent reflections
2420 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.100
S = 1.02
3731 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.84 (2)	1.90 (2)	2.598 (2)	139.3 (19)
C15—H15···O1^{i}	0.93	2.40	3.236 (2)	149

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Starter Fund of Southeast University for financial support towards the purchase of the CCD X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2428).

References

Bruker (2000). *SMART* (Version 5.625), *SAINT* (Version 6.01), *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Lu, J., Xu, X. N., Wang, C. D., He, J. G., Hu, Y. F. & Hu, H. W. (2002). *Tetrahedron Lett.* **43**, 8367–8369.
Wang, X. Y., Dong, Y. M., Sun, J. W., Xu, X. N., Li, R. & Hu, Y. F. (2005). *J. Org. Chem.* **70**, 1897–1900.
Xu, X. N., Lu, J., Dong, Y. M., Li, R., Ge, Z. M. & Hu, Y. F. (2004). *Tetrahedron Asymmetry* **15**, 475–479.

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supplementary materials

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3-[(2-Hydroxy-1-naphthyl)(piperidin-1-yl)methyl]benzonitrile

Z.-R. Qu

Comment

Betti-type reaction is an important method to synthesize chiral ligands and by this method many unnatural homochiral amino-phenol compounds have been obtained (Lu *et al.*, 2002; Xu *et al.*, 2004; Wang *et al.*, 2005).

Molecules of the title compound have normal geometric parameters. An intramolecular O—H···N hydrogen bond stabilizes the molecule conformation. The crystal packing is characterized by helical chains of molecules linked by C—H···O hydrogen bonds.

Experimental

2-naphthol (40 mmol, 5.77 g), 3-formylbenzonitrile (40 mmol, 5.25 g) and piperidine (40 mmol, 3.4 g) were added in a flask and reacted at 80 °C with stirring for one day. Then 50 ml e thanol was added to the flask and all the reactants were refluxed for five hours. After cooled to room temperature, the solution was filtered and white solid (compound I) was obtained as colorless block crystal.

Refinement

H atoms bonded to O atoms were located in a difference map and refined with distance restraints of O—H = 0.84 (2) Å, and with U_{iso}(H) = 1.2U_{eq}(O). Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

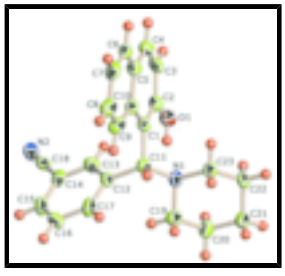

Fig. 1. The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

Fig. 2. Packing diagram of the title compound. H atoms except H1A, H15 and H11 have been omitted for clarity.

3-[(2-Hydroxy-1-naphthyl)(piperidin-1-yl)methyl]benzonitrile

Crystal data

$C_{23}H_{22}N_2O$	F_{000} = 728
M_r = 342.43	D_x = 1.199 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1875 reflections
a = 11.9008 (13) Å	θ = 2.2–21.5º
b = 15.0138 (17) Å	μ = 0.07 mm^{-1}
c = 10.8886 (13) Å	T = 291 (2) K
β = 102.867 (3)º	Block, colourless
V = 1896.7 (4) Å^3	0.30 × 0.26 × 0.24 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	3731 independent reflections
Radiation source: sealed tube	2420 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −14→14
T_{min} = 0.98, T_{max} = 0.98	k = −14→18
11353 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.100	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
3731 reflections	$\Delta\rho_{max}$ = 0.11 e Å^{-3}
238 parameters	$\Delta\rho_{min}$ = −0.11 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}
C1	0.30955 (12)	0.12699 (11)	0.28437 (15)	0.0403 (4)
C2	0.27607 (14)	0.05048 (11)	0.21554 (17)	0.0485 (4)
C3	0.32243 (16)	0.02771 (12)	0.11143 (18)	0.0553 (5)
H3	0.2952	−0.0220	0.0629	0.066*
C4	0.40741 (16)	0.07881 (12)	0.08203 (18)	0.0566 (5)
H4	0.4403	0.0615	0.0159	0.068*
C5	0.44673 (14)	0.15727 (12)	0.14922 (18)	0.0497 (4)
C6	0.53715 (14)	0.20855 (12)	0.12228 (18)	0.0518 (5)
H6	0.5736	0.1897	0.0597	0.062*
C7	0.57231 (16)	0.28492 (13)	0.18571 (19)	0.0615 (5)
H7	0.6329	0.3178	0.1679	0.074*
C8	0.51596 (15)	0.31318 (13)	0.27803 (18)	0.0591 (5)
H8	0.5383	0.3665	0.3199	0.071*
C9	0.42956 (15)	0.26544 (13)	0.30865 (17)	0.0555 (5)
H9	0.3932	0.2869	0.3700	0.067*
C10	0.39372 (13)	0.18291 (11)	0.24820 (16)	0.0436 (4)
C11	0.25970 (13)	0.15140 (10)	0.39746 (16)	0.0433 (4)
H11	0.3176	0.1861	0.4564	0.052*
C12	0.15260 (14)	0.20908 (11)	0.35548 (17)	0.0460 (4)
C13	0.06387 (15)	0.18524 (12)	0.25509 (19)	0.0553 (5)
H13	0.0698	0.1330	0.2110	0.066*
C14	−0.03407 (14)	0.23828 (11)	0.21927 (17)	0.0500 (4)
C15	−0.04187 (17)	0.31443 (13)	0.28523 (19)	0.0644 (5)
H15	−0.1075	0.3496	0.2624	0.077*
C16	0.04448 (15)	0.34030 (13)	0.38410 (19)	0.0597 (5)
H16	0.0383	0.3930	0.4270	0.072*
C17	0.14176 (16)	0.28668 (11)	0.41951 (18)	0.0569 (5)
H17	0.2003	0.3035	0.4873	0.068*
C18	−0.12332 (15)	0.21210 (11)	0.11744 (19)	0.0490 (4)
C19	0.17039 (16)	0.08659 (13)	0.56160 (19)	0.0585 (5)
H19A	0.0981	0.1157	0.5243	0.070*
H19B	0.2148	0.1264	0.6242	0.070*
C20	0.14652 (16)	0.00002 (13)	0.6246 (2)	0.0622 (5)

H20A	0.1056	0.0134	0.6901	0.075*
H20B	0.0974	−0.0377	0.5627	0.075*
C21	0.25598 (17)	−0.04955 (14)	0.68138 (19)	0.0649 (5)
H21A	0.2375	−0.1063	0.7145	0.078*
H21B	0.3018	−0.0153	0.7502	0.078*
C22	0.32365 (16)	−0.06450 (13)	0.58052 (19)	0.0613 (5)
H22B	0.2810	−0.1042	0.5166	0.074*
H22A	0.3968	−0.0925	0.6177	0.074*
C23	0.34519 (14)	0.02330 (13)	0.52003 (19)	0.0553 (5)
H23A	0.3916	0.0618	0.5831	0.066*
H23B	0.3876	0.0123	0.4551	0.066*
N1	0.23443 (10)	0.06843 (9)	0.46359 (14)	0.0472 (4)
N2	−0.19638 (14)	0.19212 (12)	0.03453 (17)	0.0689 (5)
O1	0.19695 (11)	−0.00654 (8)	0.24320 (13)	0.0568 (3)
H1A	0.1741 (17)	0.0125 (14)	0.306 (2)	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0355 (7)	0.0412 (9)	0.0427 (9)	0.0043 (6)	0.0054 (7)	0.0003 (7)
C2	0.0498 (9)	0.0394 (9)	0.0551 (11)	0.0039 (8)	0.0093 (8)	0.0010 (8)
C3	0.0623 (11)	0.0405 (9)	0.0615 (12)	0.0136 (8)	0.0106 (9)	−0.0089 (8)
C4	0.0647 (11)	0.0565 (11)	0.0510 (11)	0.0148 (10)	0.0181 (9)	0.0013 (9)
C5	0.0453 (9)	0.0527 (10)	0.0539 (11)	0.0040 (8)	0.0173 (8)	0.0041 (8)
C6	0.0464 (9)	0.0604 (12)	0.0532 (11)	0.0159 (9)	0.0206 (8)	0.0172 (9)
C7	0.0581 (11)	0.0619 (13)	0.0633 (13)	−0.0099 (9)	0.0109 (10)	0.0198 (10)
C8	0.0597 (11)	0.0615 (12)	0.0533 (12)	−0.0201 (9)	0.0067 (9)	0.0022 (9)
C9	0.0548 (10)	0.0633 (12)	0.0479 (11)	−0.0189 (9)	0.0102 (8)	0.0013 (9)
C10	0.0369 (8)	0.0509 (10)	0.0411 (9)	0.0058 (7)	0.0046 (7)	0.0070 (7)
C11	0.0395 (8)	0.0406 (8)	0.0499 (10)	−0.0042 (7)	0.0098 (7)	−0.0003 (7)
C12	0.0416 (8)	0.0450 (9)	0.0558 (11)	0.0043 (7)	0.0201 (8)	0.0129 (8)
C13	0.0588 (10)	0.0454 (10)	0.0653 (12)	−0.0003 (9)	0.0217 (9)	−0.0090 (9)
C14	0.0503 (10)	0.0417 (9)	0.0596 (11)	−0.0122 (8)	0.0158 (8)	0.0164 (8)
C15	0.0689 (12)	0.0550 (12)	0.0592 (12)	0.0147 (10)	−0.0073 (10)	0.0098 (9)
C16	0.0621 (11)	0.0542 (11)	0.0633 (13)	0.0126 (9)	0.0147 (10)	−0.0117 (9)
C17	0.0643 (11)	0.0423 (10)	0.0533 (11)	−0.0030 (8)	−0.0101 (9)	0.0094 (8)
C18	0.0500 (10)	0.0491 (10)	0.0548 (11)	0.0025 (8)	0.0264 (9)	−0.0040 (8)
C19	0.0560 (10)	0.0628 (12)	0.0614 (12)	0.0023 (9)	0.0234 (9)	0.0091 (10)
C20	0.0606 (11)	0.0656 (12)	0.0610 (12)	0.0086 (10)	0.0149 (9)	0.0154 (10)
C21	0.0696 (12)	0.0693 (13)	0.0577 (12)	0.0199 (10)	0.0183 (10)	0.0159 (10)
C22	0.0634 (11)	0.0590 (11)	0.0647 (13)	0.0303 (10)	0.0213 (10)	0.0200 (10)
C23	0.0429 (9)	0.0651 (12)	0.0584 (12)	0.0137 (9)	0.0120 (8)	0.0145 (9)
N1	0.0390 (7)	0.0481 (8)	0.0547 (9)	0.0042 (6)	0.0110 (6)	0.0129 (7)
N2	0.0621 (10)	0.0778 (12)	0.0612 (11)	0.0263 (9)	0.0021 (9)	0.0027 (9)
O1	0.0627 (8)	0.0454 (7)	0.0613 (9)	−0.0108 (6)	0.0118 (6)	−0.0089 (6)

Geometric parameters (Å, °)

C1—C2	1.381 (2)	C14—C15	1.364 (3)

C1—C10	1.428 (2)	C14—C18	1.410 (3)
C1—C11	1.526 (2)	C15—C16	1.369 (3)
C2—O1	1.355 (2)	C15—H15	0.9300
C2—C3	1.409 (3)	C16—C17	1.392 (2)
C3—C4	1.363 (3)	C16—H16	0.9300
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.410 (3)	C18—N2	1.145 (2)
C4—H4	0.9300	C19—N1	1.468 (2)
C5—C6	1.406 (2)	C19—C20	1.525 (3)
C5—C10	1.418 (2)	C19—H19A	0.9700
C6—C7	1.356 (3)	C19—H19B	0.9700
C6—H6	0.9300	C20—C21	1.508 (2)
C7—C8	1.393 (3)	C20—H20A	0.9700
C7—H7	0.9300	C20—H20B	0.9700
C8—C9	1.355 (2)	C21—C22	1.516 (3)
C8—H8	0.9300	C21—H21A	0.9700
C9—C10	1.423 (2)	C21—H21B	0.9700
C9—H9	0.9300	C22—C23	1.521 (3)
C11—N1	1.502 (2)	C22—H22B	0.9700
C11—C12	1.524 (2)	C22—H22A	0.9700
C11—H11	0.9800	C23—N1	1.488 (2)
C12—C17	1.378 (2)	C23—H23A	0.9700
C12—C13	1.387 (2)	C23—H23B	0.9700
C13—C14	1.394 (2)	O1—H1A	0.84 (2)
C13—H13	0.9300		
C2—C1—C10	118.34 (15)	C14—C15—C16	121.65 (17)
C2—C1—C11	121.38 (15)	C14—C15—H15	119.2
C10—C1—C11	120.27 (14)	C16—C15—H15	119.2
O1—C2—C1	122.39 (16)	C15—C16—C17	119.09 (17)
O1—C2—C3	116.20 (15)	C15—C16—H16	120.5
C1—C2—C3	121.41 (16)	C17—C16—H16	120.5
C4—C3—C2	119.76 (17)	C12—C17—C16	120.96 (17)
C4—C3—H3	120.1	C12—C17—H17	119.5
C2—C3—H3	120.1	C16—C17—H17	119.5
C3—C4—C5	121.74 (18)	N2—C18—C14	179.0 (2)
C3—C4—H4	119.1	N1—C19—C20	110.32 (16)
C5—C4—H4	119.1	N1—C19—H19A	109.6
C6—C5—C4	122.00 (18)	C20—C19—H19A	109.6
C6—C5—C10	120.04 (17)	N1—C19—H19B	109.6
C4—C5—C10	117.95 (16)	C20—C19—H19B	109.6
C7—C6—C5	121.36 (18)	H19A—C19—H19B	108.1
C7—C6—H6	119.3	C21—C20—C19	111.99 (16)
C5—C6—H6	119.3	C21—C20—H20A	109.2
C6—C7—C8	118.79 (17)	C19—C20—H20A	109.2
C6—C7—H7	120.6	C21—C20—H20B	109.2
C8—C7—H7	120.6	C19—C20—H20B	109.2
C9—C8—C7	122.02 (19)	H20A—C20—H20B	107.9
C9—C8—H8	119.0	C20—C21—C22	109.00 (16)
C7—C8—H8	119.0	C20—C21—H21A	109.9

C8—C9—C10	120.84 (18)	C22—C21—H21A	109.9
C8—C9—H9	119.6	C20—C21—H21B	109.9
C10—C9—H9	119.6	C22—C21—H21B	109.9
C5—C10—C9	116.72 (15)	H21A—C21—H21B	108.3
C5—C10—C1	120.54 (16)	C21—C22—C23	110.69 (16)
C9—C10—C1	122.73 (15)	C21—C22—H22B	109.5
N1—C11—C12	111.81 (12)	C23—C22—H22B	109.5
N1—C11—C1	110.06 (13)	C21—C22—H22A	109.5
C12—C11—C1	110.11 (13)	C23—C22—H22A	109.5
N1—C11—H11	108.3	H22B—C22—H22A	108.1
C12—C11—H11	108.3	N1—C23—C22	110.76 (14)
C1—C11—H11	108.3	N1—C23—H23A	109.5
C17—C12—C13	118.43 (15)	C22—C23—H23A	109.5
C17—C12—C11	119.65 (16)	N1—C23—H23B	109.5
C13—C12—C11	121.91 (15)	C22—C23—H23B	109.5
C12—C13—C14	121.04 (16)	H23A—C23—H23B	108.1
C12—C13—H13	119.5	C19—N1—C23	109.87 (14)
C14—C13—H13	119.5	C19—N1—C11	112.71 (13)
C15—C14—C13	118.83 (17)	C23—N1—C11	108.79 (12)
C15—C14—C18	121.33 (16)	C2—O1—H1A	109.5 (14)
C13—C14—C18	119.83 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N1	0.84 (2)	1.90 (2)	2.598 (2)	139.3 (19)
C15—H15···O1^{i}	0.93	2.40	3.236 (2)	149

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

Fig. 1

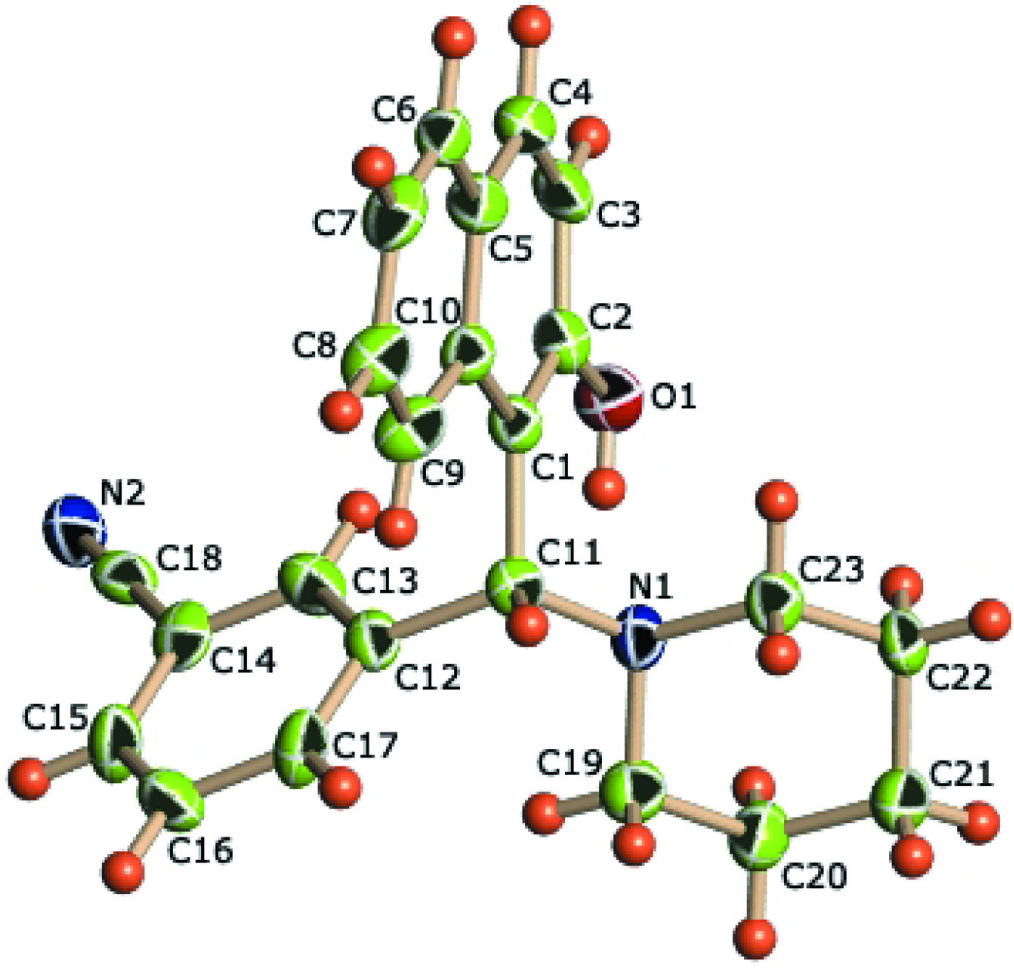
C6
C4
C7
C3
C5
C10
C2
C8
O1
C9
C1
N2
C18
C11
C13
N1
C23
C14
C12
C22
C15
C17
C19
C21
C16
C20

Fig. 2