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10-Methoxybenzo[*g*]imidazo[1,2-*a*][1,8]-naphthyridine-4-carbonitrile

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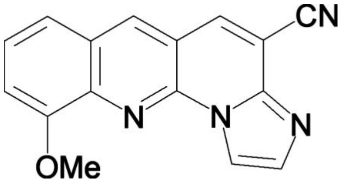
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.002 Å; R factor = 0.052; wR factor = 0.164; data-to-parameter ratio = 18.5.

In the title compound, $C_{16}H_{10}N_4O$, both the methoxy and nitrile substituents lie in the plane defined by the benzo[*g*]-imidazo[1,2-*a*]-1,8-naphthyridine ring system, resulting in a nearly planar geometry for the entire molecule (r.m.s. deviation of the non-H atoms from the mean plane is 0.044 Å). In the solid-state, the molecules form a three-dimensional polymer through intermolecular C—H···N and C—H···O hydrogen bonds. In addition, the packing mode results in stabilizing π–π stacking interactions between the asymmetric units.

Related literature

For the synthesis of the title compound and a series of similar products, see: Volovnenko *et al.* (2009). For related compounds and their antibacterial or photophysical properties, see: Kondo *et al.* (1990); Gokhale & Seshadri (1987); Rajagopal & Seshadri (1991); Vijila *et al.* (2000). For the solid-state structures of other imidazonaphthyridine derivatives, see: Fun *et al.* (1996); Sivakumar *et al.* (1996*a*,*b*); Muthamizhchelvan *et al.* (2005*a*,*b*). For general metrical features within organic compounds, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{10}N_4O$
M_r = 274.28
Monoclinic, $P2_1/c$
a = 7.710 (2) Å
b = 11.970 (2) Å
c = 13.340 (3) Å
β = 93.55 (3)°
V = 1228.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 180 K
0.40 × 0.40 × 0.35 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{\min}$ = 0.95, $T_{\max}$ = 0.97
45253 measured reflections
3532 independent reflections
2507 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.164
S = 1.08
3532 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.33 e Å^{-3}
$\Delta\rho_{\min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1$^{\rm i}$	0.93	2.50	3.366 (3)	156
C3—H3···N1$^{\rm ii}$	0.93	2.62	3.394 (2)	141

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

Table 2
π–π stacking interactions (Å, °).

$Cg_{\rm i}$	$Cg_{\rm j}$	Centroid distance	Interplanar spacing $^{\rm i}$	$\alpha^{\rm ii}$	$\gamma^{\rm iii}$
$Cg1$	$Cg2^{\rm iv}$	3.487 (2)	3.322	2.68	15.42
$Cg2$	$Cg1^{\rm iv}$	3.487 (2)	3.361	2.68	17.68
$Cg3$	$Cg3^{\rm iv}$	3.710 (2)	3.382	0.00	24.27
$Cg1$	$Cg4^{\rm v}$	3.689 (2)	3.336	5.01	25.28
$Cg4$	$Cg1^{\rm v}$	3.689 (2)	3.397	5.01	22.98

Notes: (i) perpendicular distance between the centroid of the first ring and the plane of the second ring; (ii) dihedral angle between the plane of the first ring and the plane of the second ring; (iii) angle between the centroid of the first ring and the normal to the plane of the second ring; (iv) symmetry code: $-x, -y, 1-z$; (v) symmetry code: $1-x, -y, 1-z$. $Cg1$ is the centroid of atoms N1/C1/N2/C13/C14, $Cg2$ is the centroid of atoms N3/C12/C4–C6/C11, $Cg3$ is the centroid of atoms N2/C1–C4/C12 and $Cg4$ is the centroid of atoms C6–C11.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker (2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2229).

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Acta Cryst. (2009). E**65**, o2524–o2525 Tarasov *et al.* • $C_{16}H_{10}N_4O$ **o2525**

supplementary materials

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10-Methoxybenzo[*g*]imidazo[1,2-*a*][1,8]naphthyridine-4-carbonitrile

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Comment

New heterocyclic nitrogen-containing systems are always of great interest to synthetic as well as pharmaceutical organic chemists. We have recently reported an efficient and versatile route to benzo[*g*]imidazo[1,2-*a*]-1,8-naphthyridines upon thermal reaction of 2-chloroquinoline-3-carbaldehydes with 1-substitued hetarylacetonitriles (Volovnenko *et al.*, 2009). Here we report the crystal structure of the one of synthesized compound, namely, 10-methoxybenzo[*g*]imidazo[1,2-*a*]-1,8-naphthyridine-4-carbonitrile. It has been reported that products with similar structures possess not only antibacterial activity (Kondo *et al.*, 1990) but also interesting photophysical properties (Gokhale & Seshadri, 1987; Rajagopal & Seshadri, 1991; Vijila *et al.*, 2000).

Fig. 1 shows a perspective view of the asymetric unit of the title compound, including the labelling scheme. Selected bond distances and angles are given in Table 1. The benzo[*g*]imidazo[1,2-*a*]-1,8-naphthyridine core is almost planar (RMS deviation of C1>C14 and N1>N3 from mean plane is 0.035 Å). In addition, both methoxy and carbonitrile substituents attached to C(2) and C(11), respectively, are oriented in such a way that they both lay in heterocyle plane granting a nearly planar geometry to the entire molecule (RMS deviation of the all non-hydrogen atoms from mean plane is 0.044 Å). Bond distances and angles in the title compound are normal (Allen *et al.*, 1987) and compare well with other imidazonaphtyridines derivatives (Fun *et al.*, 1996; Sivakumar *et al.*.1996*a*,b; Muthamizhchelvan *et al.*, 2005*a*,b).

The crystal structure is stabilized by C—H···N and C—H···O intermolecular hydrogen bonds (Table 1) forming a three dimensional polymeric structure (Figure 2). In addition, the asymmetric units are seen to be stacked along the (100) axis with relatively short interplanar distances (Table 3) possibly allowing additional stabilization through π–π stacking interactions (Figure 3).

Experimental

The title compound was synthesized by the reaction of 2-chloro-8-methoxyquinoline-3-carbaldehyde (2 mmol) with (1-benzyl-1*H*-imidazol-2-yl)acetonitrile (2 mmol) in dimethylformamide (3 ml). After refluxing for 1 h, the reaction mixture was left to stand overnight. The resulting crude solid was filtered, washed twice with acetone (10 ml) and dried. Yield: 96%. Crystals suitable for X-ray analysis were obtained by slow crystallization from hot dimethylformamide.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.96 Å (methyl) or 0.93 Å (aromatic) with $U_{iso}(H) = 1.2U_{eq}(C_{arom})$ or $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$.

Figures

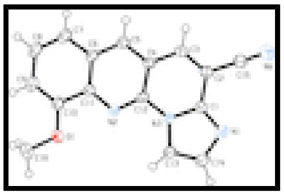


Fig. 1. A perspective view of the title compound, with 50% probability displacement ellipsoids for non-H atoms.

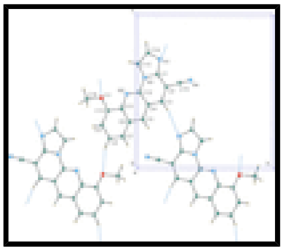


Fig. 2. A packing diagram for the title compound, evidencing C—H···N et C—H···O hydrogen bonds (blue dotted lines).

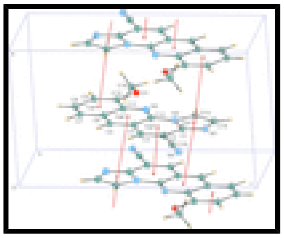


Fig. 3. A packing diagram for the title compound, evidencing π-π stacking interactions (red dotted lines).

10-Methoxybenzo[*g*]imidazo[1,2-*a*][1,8]naphthyridine-4-carbonitrile

Crystal data

$C_{16}H_{10}N_4O$

$M_r = 274.28$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.710$ (2) Å

$b = 11.970$ (2) Å

$c = 13.340$ (3) Å

$\beta = 93.55$ (3)°

$V = 1228.8$ (5) Å^3

$Z = 4$

$F_{000} = 568$

$D_x = 1.483$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9999 reflections

$\theta = 2.7$–34.9°

$\mu = 0.10$ mm^{-1}

$T = 180$ K

Block, brown

0.40 × 0.40 × 0.35 mm

Data collection

Bruker APEXII
diffractometer

Radiation source: sealed tube

Monochromator: graphite

$T = 180$ K

φ scans

Absorption correction: multi-scan
(SADABS; Bruker, 2007)

3532 independent reflections

2507 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.050$

$\theta_{\rm max} = 29.8$°

$\theta_{\rm min} = 2.3$°

$h = -10\rightarrow10$

$T_{min} = 0.95$, $T_{max} = 0.97$	$k = -16 \rightarrow 16$
45253 measured reflections	$l = -18 \rightarrow 18$

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
$wR(F^2) = 0.164$	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 1.0259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
3532 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
191 parameters	$\Delta\rho_{min} = -0.33$ 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 $F^2 > \sigma(F^2)$ 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	0.1160 (2)	0.16186 (14)	0.60289 (12)	0.0239 (3)
C2	0.0449 (2)	0.22693 (14)	0.51977 (13)	0.0257 (3)
C3	0.0661 (2)	0.19331 (15)	0.42439 (13)	0.0264 (4)
H3	0.0201	0.2358	0.3708	0.032*
C4	0.1593 (2)	0.09249 (14)	0.40567 (12)	0.0239 (3)
C5	0.1800 (2)	0.05231 (15)	0.31021 (13)	0.0271 (4)
H5	0.1352	0.0921	0.2546	0.033*
C6	0.2686 (2)	−0.04838 (15)	0.29677 (12)	0.0262 (4)
C7	0.2865 (3)	−0.09560 (17)	0.20044 (13)	0.0339 (4)
H7	0.2407	−0.0588	0.1433	0.041*
C8	0.3705 (3)	−0.19467 (18)	0.19165 (15)	0.0378 (5)
H8	0.3800	−0.2260	0.1284	0.045*
C9	0.4435 (3)	−0.25045 (16)	0.27749 (15)	0.0344 (4)
H9	0.5029	−0.3173	0.2698	0.041*
C10	0.4285 (2)	−0.20791 (14)	0.37173 (13)	0.0268 (4)
C11	0.3374 (2)	−0.10535 (14)	0.38426 (12)	0.0232 (3)

C12	0.2307 (2)	0.02653 (14)	0.48692 (12)	0.0222 (3)
C13	0.2521 (2)	0.01703 (15)	0.67504 (13)	0.0282 (4)
H13	0.3126	−0.0494	0.6869	0.034*
C14	0.1924 (3)	0.08839 (16)	0.74444 (14)	0.0329 (4)
H14	0.2065	0.0773	0.8135	0.039*
C15	−0.0484 (2)	0.32689 (16)	0.54198 (14)	0.0307 (4)
C16	0.5661 (3)	−0.36456 (17)	0.45063 (18)	0.0399 (5)
H16A	0.4794	−0.4139	0.4207	0.060*
H16B	0.6029	−0.3913	0.5164	0.060*
H16C	0.6639	−0.3621	0.4095	0.060*
N1	0.1082 (2)	0.17940 (14)	0.69986 (11)	0.0311 (3)
N2	0.31704 (18)	−0.06777 (12)	0.47856 (10)	0.0231 (3)
N3	0.20387 (18)	0.06431 (12)	0.58360 (10)	0.0233 (3)
N4	−0.1221 (3)	0.40663 (16)	0.55947 (15)	0.0451 (5)
O1	0.49489 (18)	−0.25543 (11)	0.45838 (10)	0.0338 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0238 (8)	0.0251 (8)	0.0228 (8)	−0.0042 (6)	0.0013 (6)	0.0000 (6)
C2	0.0248 (8)	0.0261 (8)	0.0263 (8)	−0.0034 (6)	0.0010 (6)	0.0034 (6)
C3	0.0277 (8)	0.0265 (8)	0.0248 (8)	−0.0023 (6)	−0.0009 (6)	0.0060 (6)
C4	0.0253 (8)	0.0247 (8)	0.0215 (7)	−0.0043 (6)	0.0006 (6)	0.0037 (6)
C5	0.0313 (9)	0.0297 (8)	0.0201 (7)	−0.0062 (7)	−0.0001 (6)	0.0037 (6)
C6	0.0294 (8)	0.0281 (8)	0.0211 (8)	−0.0089 (7)	0.0025 (6)	−0.0002 (6)
C7	0.0440 (11)	0.0377 (10)	0.0205 (8)	−0.0124 (8)	0.0049 (7)	−0.0007 (7)
C8	0.0487 (12)	0.0401 (11)	0.0257 (9)	−0.0111 (9)	0.0107 (8)	−0.0086 (8)
C9	0.0401 (10)	0.0298 (9)	0.0344 (10)	−0.0070 (8)	0.0113 (8)	−0.0078 (7)
C10	0.0292 (8)	0.0236 (8)	0.0282 (8)	−0.0061 (6)	0.0051 (7)	−0.0006 (6)
C11	0.0249 (8)	0.0237 (8)	0.0213 (7)	−0.0074 (6)	0.0031 (6)	−0.0008 (6)
C12	0.0224 (7)	0.0242 (7)	0.0200 (7)	−0.0060 (6)	0.0011 (6)	0.0013 (6)
C13	0.0329 (9)	0.0296 (8)	0.0218 (8)	−0.0015 (7)	−0.0018 (6)	0.0046 (6)
C14	0.0385 (10)	0.0368 (10)	0.0234 (8)	−0.0033 (8)	0.0014 (7)	0.0012 (7)
C15	0.0314 (9)	0.0321 (9)	0.0285 (9)	−0.0003 (7)	0.0019 (7)	0.0026 (7)
C16	0.0434 (11)	0.0258 (9)	0.0509 (13)	0.0023 (8)	0.0056 (9)	−0.0012 (8)
N1	0.0360 (8)	0.0337 (8)	0.0239 (7)	−0.0032 (6)	0.0048 (6)	−0.0023 (6)
N2	0.0261 (7)	0.0234 (7)	0.0199 (6)	−0.0041 (5)	0.0016 (5)	0.0002 (5)
N3	0.0260 (7)	0.0237 (7)	0.0199 (6)	−0.0025 (5)	0.0000 (5)	0.0009 (5)
N4	0.0515 (11)	0.0399 (10)	0.0444 (10)	0.0086 (9)	0.0066 (8)	−0.0008 (8)
O1	0.0423 (8)	0.0264 (6)	0.0330 (7)	0.0034 (6)	0.0050 (6)	0.0004 (5)

Geometric parameters (Å, °)

C1—N1	1.315 (2)	C9—C10	1.368 (3)
C1—N3	1.382 (2)	C9—H9	0.9300
C1—C2	1.436 (2)	C10—O1	1.360 (2)
C2—C3	1.354 (2)	C10—C11	1.429 (2)
C2—C15	1.436 (3)	C11—N2	1.354 (2)
C3—C4	1.434 (2)	C12—N2	1.319 (2)

C3—H3	0.9300	C12—N3	1.394 (2)
C4—C5	1.380 (2)	C13—C14	1.361 (3)
C4—C12	1.424 (2)	C13—N3	1.375 (2)
C5—C6	1.402 (3)	C13—H13	0.9300
C5—H5	0.9300	C14—N1	1.384 (3)
C6—C7	1.418 (2)	C14—H14	0.9300
C6—C11	1.425 (2)	C15—N4	1.142 (3)
C7—C8	1.360 (3)	C16—O1	1.423 (2)
C7—H7	0.9300	C16—H16A	0.9600
C8—C9	1.412 (3)	C16—H16B	0.9600
C8—H8	0.9300	C16—H16C	0.9600

N1—C1—N3	111.76 (15)	O1—C10—C11	114.95 (15)
N1—C1—C2	129.36 (16)	C9—C10—C11	119.84 (17)
N3—C1—C2	118.86 (15)	N2—C11—C6	122.89 (16)
C3—C2—C1	120.12 (16)	N2—C11—C10	118.69 (15)
C3—C2—C15	122.18 (16)	C6—C11—C10	118.41 (15)
C1—C2—C15	117.70 (16)	N2—C12—N3	117.42 (14)
C2—C3—C4	120.31 (16)	N2—C12—C4	125.71 (15)
C2—C3—H3	119.8	N3—C12—C4	116.86 (15)
C4—C3—H3	119.8	C14—C13—N3	105.12 (16)
C5—C4—C12	116.60 (16)	C14—C13—H13	127.4
C5—C4—C3	122.82 (15)	N3—C13—H13	127.4
C12—C4—C3	120.55 (15)	C13—C14—N1	111.80 (16)
C4—C5—C6	120.19 (16)	C13—C14—H14	124.1
C4—C5—H5	119.9	N1—C14—H14	124.1
C6—C5—H5	119.9	N4—C15—C2	179.7 (2)
C5—C6—C7	122.25 (17)	O1—C16—H16A	109.5
C5—C6—C11	117.77 (15)	O1—C16—H16B	109.5
C7—C6—C11	119.95 (17)	H16A—C16—H16B	109.5
C8—C7—C6	119.94 (18)	O1—C16—H16C	109.5
C8—C7—H7	120.0	H16A—C16—H16C	109.5
C6—C7—H7	120.0	H16B—C16—H16C	109.5
C7—C8—C9	120.70 (18)	C1—N1—C14	104.37 (15)
C7—C8—H8	119.6	C12—N2—C11	116.81 (14)
C9—C8—H8	119.6	C13—N3—C1	106.94 (14)
C10—C9—C8	121.13 (19)	C13—N3—C12	129.77 (15)
C10—C9—H9	119.4	C1—N3—C12	123.28 (14)
C8—C9—H9	119.4	C10—O1—C16	116.67 (15)
O1—C10—C9	125.21 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.93	2.50	3.366 (3)	156
C3—H3···N1^{ii}	0.93	2.62	3.394 (2)	141

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

Table 2

π–π stacking interactions (Å, °)

Cg$_i$	*Cg*$_j$	Centroid distance	Interplanar spacing ^{i}	α^{ii}	γ^{iii}
*Cg*1	*Cg*2^{iv}	3.487 (2)	3.322	2.68	15.42
*Cg*2	*Cg*1^{iv}	3.487 (2)	3.361	2.68	17.68
*Cg*3	*Cg*3^{iv}	3.710 (2)	3.382	0.00	24.27
*Cg*1	*Cg*4^{v}	3.689 (2)	3.336	5.01	25.28
*Cg*4	*Cg*1^{v}	3.689 (2)	3.397	5.01	22.98

Notes: (i) perpendicular distance between the centroid of the first ring and the plane of the second ring; (ii) dihedral angle between the plane of the first ring and the plane of the second ring; (iii) angle between the centroid of the first ring and the normal to the plane of the second ring; (iv) symmetry code: -x, -y, 1-z; (v) symmetry code: 1 - x, -y,1 - z. *Cg*1 is the centroid of atoms N1/C1/N2/C13/C14, *Cg*2 is the centroid of atoms N3/C12/C4–C6/C11, *Cg*3 is the centroid of atoms N2/C1–C4/C12 and *Cg*4 is the centroid of atoms C6–C11.

Fig. 1

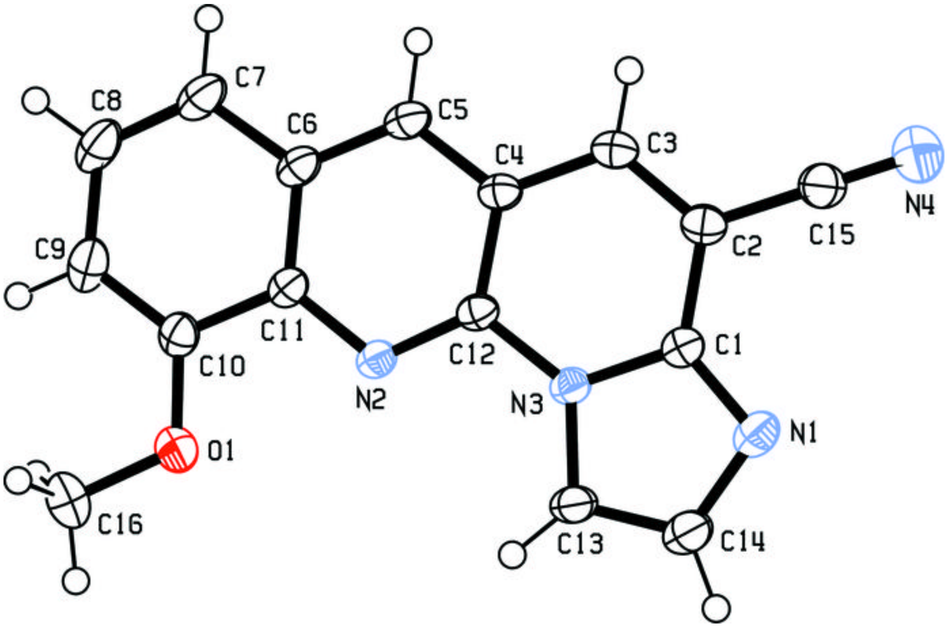


Fig. 2

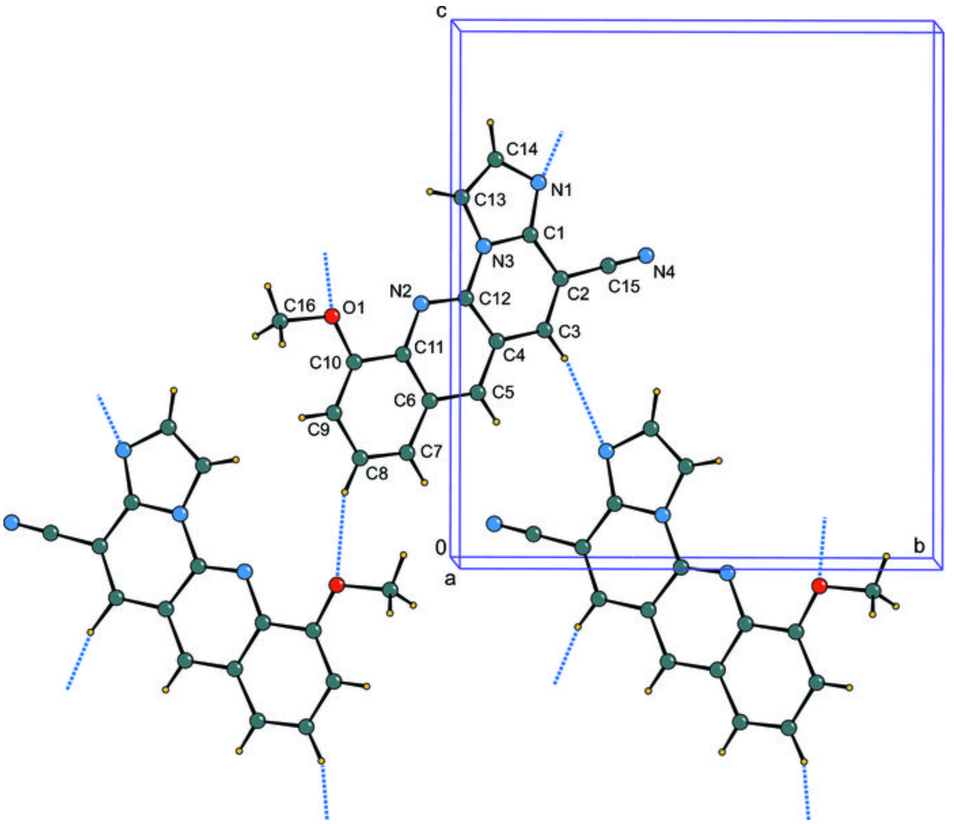
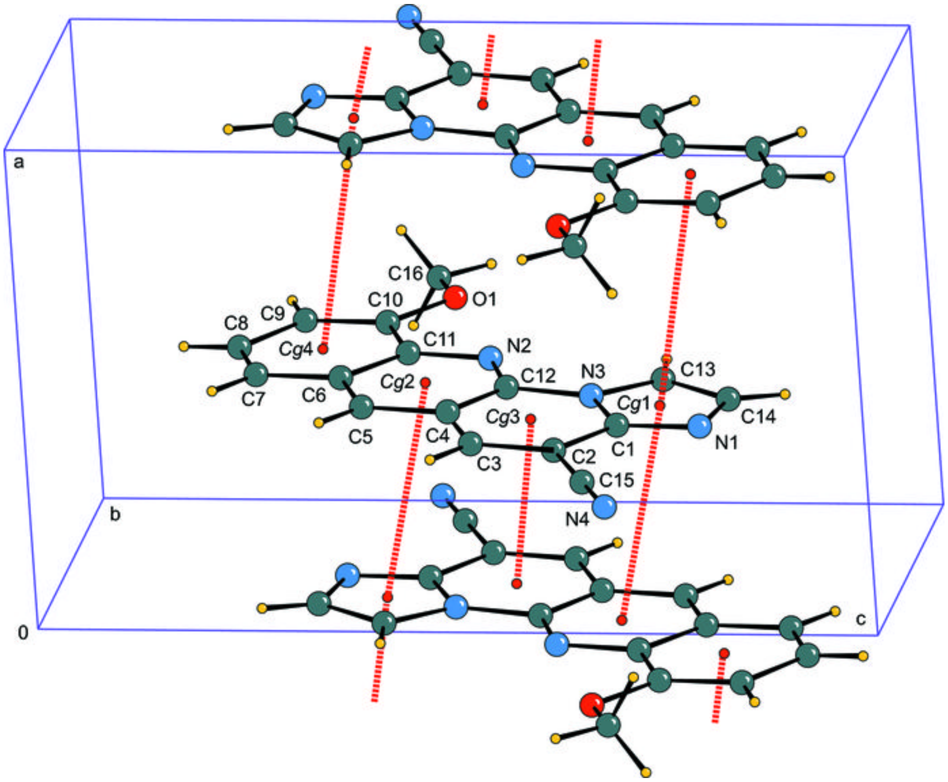

c
C14
N1
C13
C1
N3
C2
C15
N4
N2
C12
C16
O1
C3
C11
C10
C4
C6
C5
C9
C7
C8
0
a
b

Fig. 3


a
b
0
c
C16
O1
C10
C9
C8
C11
N2
Cg4
C12
N3
C13
C6
Cg2
C7
Cg1
Cg3
C14
C5
C4
C1
N1
C2
C3
C15
N4