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# 2-Amino-4-(3,4-dimethoxyphenyl)-5,6-dihydrobenzo[*h*]quinoline-3-carbonitrile–3-amino-1-(3,4-dimethoxyphenyl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile (1/19)

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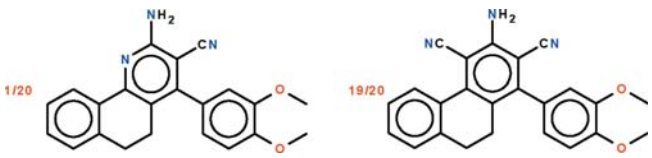
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; disorder in main residue; $R$ factor = 0.049; $wR$ factor = 0.124; data-to-parameter ratio = 15.4.

The asymmetric unit of the 1:19 title co-crystal of 2-amino-4-(3,4-dimethoxyphenyl)-5,6-dihydrobenzo[*h*]quinoline-3-carbonitrile and 3-amino-1-(3,4-dimethoxyphenyl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile, $0.05C_{22}H_{19}N_3O_2\cdot 0.95C_{24}H_{19}N_3O_2$, has the atoms of the fused-ring system and those of the amino, cyano and dimethoxyphenyl substitutents overlapped. The fused-ring system is buckled owing to the ethylene linkage in the central ring with the two flanking aromatic rings being twisted by 31.9 (1)°. The ring of the dimethoxyphenyl substituent is twisted by 72.4 (1)° relative to the amino- and cyano-bearing aromatic ring. In the crystal, molecules are linked by duplex amine N—H···O(methoxy) hydrogen bonds in a cyclic association [graph-set $R_2^2(7)$], generating a helical chain structure extending along [201].

## Related literature

For a similar co-crystal, see: Asiri *et al.* (2011). For graph-set analysis, see: Etter *et al.* (1990).




## Experimental

### Crystal data

$0.05C_{22}H_{19}N_3O_2\cdot 0.95C_{24}H_{19}N_3O_2$
$M_r$ = 380.22
Monoclinic, $P2_1/c$
$a$ = 8.9347 (3) Å
$b$ = 14.4915 (5) Å
$c$ = 14.7818 (6) Å
$\beta$ = 103.446 (4)°
$V$ = 1861.45 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 100 K
0.30 × 0.25 × 0.20 mm

### Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.974, $T_{max}$ = 0.983
9240 measured reflections
4160 independent reflections
3146 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.124
$S$ = 1.04
4160 reflections
270 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H1···O1$^{i}$ | 0.95 (2) | 2.24 (2) | 2.927 (2) | 129 (2) |
| N3—H2···O2$^{i}$ | 0.92 (2) | 2.25 (2) | 2.987 (2) | 136 (2) |

Symmetry code: (i) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2146).

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