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Crystal structure of 6-amino-8-(4-isopropylphenyl)-2-methyl-2,3,8,8a-tetrahydroisoquinoline-5,7,7(1*H*)-tricarbonitrile-ethanol (1/1), C₂₄H₂₉N₅O

The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.26 × 0.24 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.5 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5828, 3963, 0.027
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2065
$N(\text{param})_{\text{refined}}$:	272
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.5152(3)	−0.0059(3)	0.28650(19)	0.1053(8)
H1	0.549377	0.030107	0.359321	0.158*
N1	−0.1560(3)	0.9145(3)	0.0206(2)	0.0797(8)
N2	0.1867(3)	0.8924(3)	0.1333(2)	0.0710(7)
H2A	0.159829	0.945601	0.096842	0.085*
H2B	0.279398	0.902183	0.151252	0.085*
N3	0.2934(3)	0.6391(3)	0.1194(3)	0.0872(9)
N4	0.3160(3)	0.8493(3)	0.4510(2)	0.0774(7)
N5	−0.3552(3)	0.4769(3)	0.2608(2)	0.0705(7)
C1	−0.1154(3)	0.8509(3)	0.0739(2)	0.0612(8)
C2	−0.0616(3)	0.7701(3)	0.1389(2)	0.0546(7)
C3	0.0853(3)	0.7953(3)	0.1619(2)	0.0525(7)
C4	0.1433(3)	0.7048(3)	0.2229(2)	0.0522(7)
C5	0.2351(3)	0.6720(3)	0.1689(3)	0.0626(8)
C6	0.2462(3)	0.7871(3)	0.3524(3)	0.0571(7)
C7	0.0023(3)	0.5592(3)	0.2050(2)	0.0519(7)
H7	−0.057996	0.508691	0.117682	0.062*
C8	−0.1087(3)	0.5853(3)	0.2433(2)	0.0547(7)
H8	−0.048921	0.642498	0.329185	0.066*
C9	−0.1690(3)	0.6674(3)	0.1746(2)	0.0563(7)
C10	−0.3151(3)	0.6437(3)	0.1487(2)	0.0698(8)
H10	−0.347805	0.699127	0.108776	0.084*
C11	−0.4274(3)	0.5361(4)	0.1791(3)	0.0778(9)
H11A	−0.473405	0.579253	0.215462	0.093*

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Abstract

C₂₄H₂₉N₅O, triclinic, $P\bar{1}$ (no. 2), $a = 10.352(9)$ Å, $b = 10.911(10)$ Å, $c = 12.480(6)$ Å, $\alpha = 97.33(2)^\circ$, $\beta = 110.29(2)^\circ$, $\gamma = 115.353(15)^\circ$, $V = 1129.6(15)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0614$, $wR_{\text{ref}}(F^2) = 0.1855$, $T = 296(2)$ K.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H11B	−0.513741	0.459021	0.105391	0.093*
C12	−0.2487(3)	0.4470(3)	0.2274(3)	0.0683(8)
H12A	−0.305556	0.385451	0.143905	0.082*
H12B	−0.210776	0.397240	0.277753	0.082*
C13	−0.4743(4)	0.3524(4)	0.2684(3)	0.1008(12)
H13A	−0.423111	0.315078	0.323351	0.151*
H13B	−0.537194	0.378032	0.297018	0.151*
H13C	−0.542281	0.280822	0.189859	0.151*
C14	0.0586(3)	0.4662(3)	0.2603(2)	0.0534(7)
C15	0.0585(3)	0.3590(3)	0.1893(3)	0.0669(8)
H15	0.019544	0.343433	0.106620	0.080*
C16	0.1133(3)	0.2747(3)	0.2354(3)	0.0740(9)
H16	0.114004	0.205437	0.184260	0.089*
C17	0.1664(3)	0.2902(3)	0.3542(3)	0.0691(8)
C18	0.1653(3)	0.3953(3)	0.4276(3)	0.0703(8)
H18	0.201424	0.408154	0.509807	0.084*
C19	0.1113(3)	0.4821(3)	0.3807(2)	0.0607(7)
H19	0.110825	0.551784	0.431683	0.073*
C20	0.2240(4)	0.1940(4)	0.4041(4)	0.0988(12)
H20	0.240754	0.148473	0.341227	0.119*
C21	0.3841(5)	0.2767(5)	0.5129(4)	0.1153(14)
H21A	0.457686	0.351414	0.495400	0.173*
H21B	0.373674	0.318248	0.579732	0.173*
H21C	0.423361	0.213269	0.533084	0.173*
C22	0.1035(5)	0.0788(5)	0.4193(5)	0.1425(18)
H22A	0.005217	0.031577	0.346006	0.214*
H22B	0.137045	0.011384	0.437624	0.214*
H22C	0.087358	0.116364	0.484272	0.214*
C23	0.6243(10)	0.0189(9)	0.1551(8)	0.234(3)
H23A	0.715833	0.029601	0.144903	0.351*
H23B	0.530186	−0.066749	0.094731	0.351*
H23C	0.612707	0.100427	0.146912	0.351*
C24	0.6431(6)	0.0102(7)	0.2608(5)	0.163(2)
H24A	0.740108	0.096046	0.320747	0.195*
H24B	0.657724	−0.070853	0.268652	0.195*

Source of material

A mixture of *N*-methyl-4-piperidone (10 mmol), 4-isopropylbenzaldehyde (10 mmol) and malononitrile (20 mmol) in ethanol (100 mL) was refluxed for 2–3 h. The precipitates were filtered off, washed with ice-cooled water and ethanol.

Experimental details

H atoms bonded to C and N atoms were positioned geometrically and refined using a riding model, with C–H = 0.93/0.96/

0.97 Å and N–H = 0.86 Å with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ and 1.2 times $U_{\text{eq}}(\text{N})$.

Discussion

Tetrahydroisoquinoline derivatives is one of the most commonly encountered heterocycles and plays an important effect in the field of medicine [4], which is also true for the amini derivative [5]. An osteosarcoma (OS) or osteogenic sarcoma (OGS) is a cancerous tumor in a bone, specifically, it is an aggressive malignant neoplasm that arises from primitive transformed cells of mesenchymal origin and that exhibits osteoblastic differentiation and produces malignant osteoid. Osteosarcoma is the most common histological form of primary bone cancer. It is most prevalent in teenagers and young adults. Recent research has also indicated that the use of tetraquinolines is an effective treatment to shrink OS and control symptoms.

From the diagram of the asymmetric unit including the atomic numbering scheme of the title compound (*cf.* the figure), we can see an ethanol solvent molecule incorporated in the asymmetric unit. In the crystal structure of the title compound, the six-membered carbon ring is typically folded and the adjacent six-membered ring containing one nitrogen atom also adopts a flattened chair conformation. The bond lengths are all in their normal ranges and they are similar with the known compound 6-amino-8-(3,4-dimethylphenyl)-2-methyl-2,3,8,8a-tetrahydro-1*H*-isoquinoline-5,7,7-tricarbonitrile [6].

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