

Product Information

Cytochrome P450 inhibitor, TOK-001, Purity ≥98%

Cat. No.: X24-08-YM385

Size: 5 mg; 10 mg; 50 mg; 100 mg

MDL: MFCD16660907

CAS Number: 851983-85-2

Compound CID: 11188409

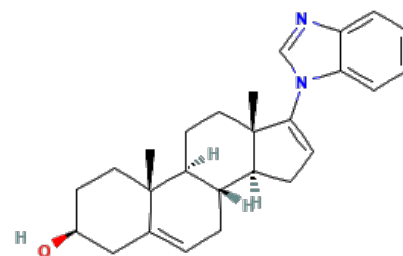
Synonym: 851983-85-2; VN/124-1; Galeterone;

(3*S*,8*R*,9*S*,10*R*,13*S*,14*S*

)-17-(Be

nzimidazol-1-yl)-

10,13-dimethyl-2,3,4,7,8,9,11,12,14,15-decahydro-1*H*-cyclopenta[*a*]phenanthren-3-ol



This product is for research use only and is not intended for diagnostic use.

Product Information

Description	TOK-001, soluble in DMSO and warmed ethanol and insoluble in water, is an effective cell metabolism inhibitor, that has the ability to prevent the pathway of metabolism by inhibiting cytochrome P450. It targets the androgen receptor and CYP17.
Molecular Weight	388.3
Molecular Formula	C ₂₆ H ₃₂ N ₂ O
Targets	Androgen Receptor: 384 nM; CYP17: 300 nM
IUPAC Name	(3 <i>S</i> ,8 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> ,13 <i>S</i> ,14 <i>S</i>)-17-(Benzimidazol-1-yl)-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-ol
InChI	InChI=1S/C26H32N2O/c1-25-13-11-18(29)15-17(25)7-8-19-20-9-10-24(26(20,2)14-12-21(19)25)28-16-27-22-5-3-4-6-23(22)28/h3-7,10,16,18-21,29H,8-9,11-15H2,1-2H3/t18-,19-,20-,21-,25-,26-/m0/s1
InChI Key	ZCIGNRJZKPOIKD-CQXVEOKZSA-N
Canonical SMILES	CC(C)C1=NC(=CS1)CN(C)C(=O)NC(CCN2CCOCC2)C(=O)NC(CCC(CC3=CC=CC=C3)NC(=O)OC4=CN=CS4)CC5=CC=CC=C5
Isomeric SMILES	CC(C)C1=NC(=CS1)CN(C)C(=O)N[C@@H](CCN2CCOCC2)C(=O)N[C@H](CC[C@H](CC3=CC=CC=C3)NC(=O)OCC4=CN=CS4)CC5=CC=CC=C5
Form	Lyophilized powder
Purity	≥98%



Titer	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects
Solubility	<i>In vitro</i> : DMSO: 21 mg/mL (54.04 mM); Water: insoluble; Ethanol (warmed): 36 mg/mL (92.65 mM); <i>In vivo</i> : 0.5% hydroxyethyl cellulose, 28 mg/mL
Stability	In its lyophilized form, the chemical remains stable for 36 months.
Quality Level	Research grade
Applications	TOK-001 is a metabolism inhibitor that plays a key role in blocking the effects of androgens, which are hormones that drive prostate cancer cell growth.
Storage	Store at -20°C, and keep desiccated.
