



Product Information

CDK inhibitor THZ531, Purity ≥98%

Cat. No.: X24-05-ZQ786

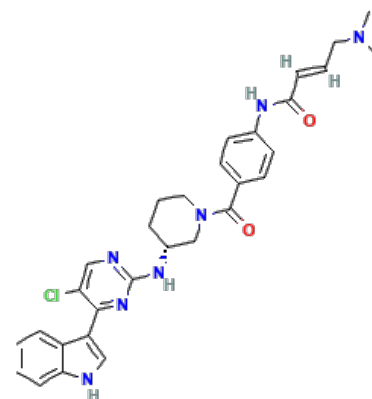
Size: 5 mg; 10 mg; 50 mg; 100 mg

CAS Number: 1702809-17-3

Compound CID: 118025540

Synonym: 1702809-17-3; THZ-531; THZ 531; CDK inhibitor

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



Product Information

Description	THZ531, soluble in DMSO and ethanol and insoluble in water, is an CDK kinase inhibitor that disrupts cell division processes.
Molecular Weight	558.08
Molecular Formula	C ₃₀ H ₃₂ ClN ₇ O ₂
IUPAC Name	(E)-N-[4-[(3R)-3-[[5-chloro-4-(1H-indol-3-yl)pyrimidin-2-yl]amino]piperidine-1-carbonyl]phenyl]-4-(dimethylamino)but-2-enamide
InChI	InChI=1S/C30H32ClN7O2/c1-37(2)15-6-10-27(39)34-21-13-11-20(12-14-21)29(40)38-16-5-7-22(19-38)35-30-33-18-25(31)28(36-30)24-17-32-26-9-4-3-8-23(24)26/h3-4,6,8-14,17-18,22,32H,5,7,15-16,19H2,1-2H3,(H,34,39)(H,33,35,36)/b10-6+/t22-/m1/s1
InChI Key	RUBYHLPRZRMTJO-MOVYNIQHSA-N
Canonical SMILES	CN(C)CC=CC(=O)NC1=CC=C(C=C1)C(=O)N2CCCC(C2)NC3=NC=C(C(=N3)C4=CNC5=CC=CC=C54)Cl
Isomeric SMILES	CN(C)C/C=C/C(=O)NC1=CC=C(C=C1)C(=O)N2CCC[C@H](C2)NC3=NC=C(C(=N3)C4=CNC5=CC=CC=C54)Cl
Form	Lyophilized powder
Purity	≥98%
Solubility	DMSO: 95 mg/mL (170.22 mM); Water: Insoluble; Ethanol: 95 mg/mL (170.22 mM)
Identity	Confirmed by NMR/HPLC/MS.
Stability	The product is stable for three years when stored at the recommended temperature in lyophilized powder.
Applications	THZ531 can be used in research on its covalent inhibition of CDK12/13, which are involved in



transcription regulation and DNA damage response.

Storage

Store at -20°C.
