MOLNOVA
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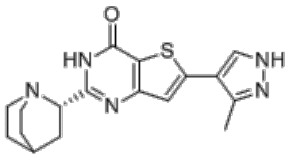
Datasheet (Version 1.0)

Product Name	:	TAK-931
Synonyms	:	Simurosertib;TAK931
Cat No.	:	M11316
CAS Number	:	1330782-76-7
Molecular Formula	:	C17H19N5OS
Formula Weight	:	341.43
Chemical Name	:	Thieno[3,2-d]pyrimidin-4(3H)-one, 2-(2S)-1-azabicyclo[2.2.2]oct-2-yl-6-(3-methyl-1H-pyrazol-4-yl)-
Description	:	TAK-931 (Simurosertib) is a potent, selective, ATP competitive and orally bioavailable inhibitor of Cdc7 with IC50 of <0.3 nM; prevents the initiation of DNA replication during mitosis, which causes cell cycle arrest and induces apoptosis, demonstrates antiproliferative activity with cancer cell lines and tumor growth inhibition (TGI) in murine ectopic xenograft models. Colon Cancer,Phase 2 Clinical
Pathway	:	Angiogenesis
Target	:	CDK
Receptor	:	CDK
Solubility	:	DMSO : 75 mg/mL 219.66 mM
SMILES	:	O=C1C2=C(C=C(C3=CNN=C3C)S2)N=C([C@H]4N(CC5)CCC5C4)N1
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	



1. Charles Locuson, et al. Abstract 5041: Translational pharmacokinetic-pharmacodynamic xenograft model for TAK-931, a small molecule cell division cycle 7 (CDC7) kinase inhibitor. AACR.| 2. Kenichi Iwai, et al. Abstract 3073: Potential predictive biomarkers of clinical responses for a novel CDC7-selective inhibitor TAK-931. AACR.