MOLNOVA
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Datasheet (Version 1.0)

Product Name	:	ZINC05007751
Synonyms	:	——
Cat No.	:	M28948
CAS Number	:	591239-68-8
Molecular Formula	:	C18H12N2O3
Formula Weight	:	304.3
Chemical Name	:	——
Description	:	ZINC05007751 is an effective inhibitor of NIMA-related kinase NEK6 (IC50 = 3.4 μM). ZINC05007751 is very selective against NEK1 and NEK6 with no significant activity observed against NEK2, NEK7, and NEK9.(In Vitro):In ovarian cancer cells PEO1, ZINC05007751 induced perturbation of the cell cycle. ZINC05007751 showed synergism with Cisplatin, resulting in a significant reduction of Cisplatin IC50 from 7.9 to 0.1??μM, with a combination of ZINC05007751 (44?μM)?+?Cisplatin (10?μM) exhibiting the greatest synergistic effect. ZINC05007751 (6 μM-190 μM; 24 hours) inhibited the growth of MDA-MB-231, PEO1, NCI-H1299, and HCT-15 with IC50 below 100?μM.
Pathway	:	MAPK/ERK Signaling
Target	:	p38 MAPK
Receptor	:	ATX (autotaxin)
Solubility	:	——
SMILES	:	CC1=C(C#N)C(O)=NC(=O)\C1=C/c1ccc(o1)-c1ccccc1
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	

1.LEE, Dae Yon, et al. NOVEL COMPOUNDS AS AUTOTAXIN INHIBITORS AND PHARMACEUTICAL COMPOSITIONS COMPRISING THE SAME. Patent O2018212534A1