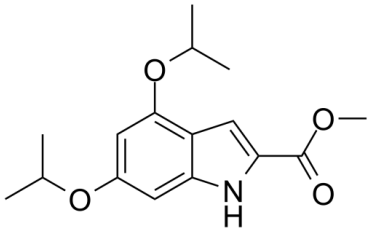
Data Sheet

Product Name:	XST-14
Cat. No.:	CS-0139563
CAS No.:	2607143-50-8
Molecular Formula:	$C_{16}H_{21}NO_4$
Molecular Weight:	291.34
Target:	ALK; CaMK; p38 MAPK; TGF-β Receptor; ULK
Pathway:	Autophagy; MAPK/ERK Pathway; Neuronal Signaling; Protein Tyrosine Kinase/RTK; TGF-beta/Smad
Solubility:	DMSO : 250 mg/mL (858.10 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

XST-14 is a potent, competitive and highly selective **ULK1** inhibitor with an **IC_{50}** of 26.6 nM. XST-14 induces **autophagy** inhibition by reducing the phosphorylation of the ULK1 downstream substrate. XST-14 induces **apoptosis** in hepatocellular carcinoma (HCC) cells and has antitumor effects[1]. **In Vitro:** XST-14 inhibits ULK1 (IC_{50}=13.6 nM), MAP2K1/MEK1 (IC_{50}=721.8 nM), MAPK14/p38 alpha (IC_{50}=283.9 nM), TGFBR2 (IC_{50}=809.3 nM), ACVR1/ALK2 (IC_{50}=183.8 nM), ULK2 (IC_{50}=70.9 nM) and CAMK2A (IC_{50}=66.3 nM) by the 10-point titration results from SelectScreen Kinase Profiling Services[1].

XST-14 (20-80 μM; for 24 h) leads a decrease in cell proliferation activity[1].

XST-14 (5 μM; for 24 h) induces apoptosis in HepG2 and human primary HCC cells[1].

XST-14 (5 μM; for 12 h) strongly inhibits the conversion of LC3-I to LC3-II in CHO cells stably expressing GFP-LC3[1].

XST-14 (5 μM; for 12 h) inhibits the Ser249 phosphorylation of PIK3C3 and Ser15 phosphorylation of BECN1[1].

In Vivo: XST-14 (15, 30 mg/kg/day; IP; for 4 consecutive weeks) displays anti-HCC efficacies, resulting in decreased tumor weights and suppressed tumor growth of HCC cells in nude mice[1].

XST-14 (2 mg/kg for IV; 10 mg/kg for IP) has a $T_{1/2}$ of 2.31 hours for IV and a $T_{1/2}$ of 2.69 hours for IP[1].

References:

[1]. Si-Tu Xue, et al. The role of the key autophagy kinase ULK1 in hepatocellular carcinoma and its validation as a treatment target . Autophagy. 2020 Oct;16(10):1823-1837.

CAIndexNames:

1H-Indole-2-carboxylic acid, 4,6-bis(1-methylethoxy)-, methyl ester

SMILES:

O=C(OC)C1=CC2=C(OC(C)C)C=C(OC(C)C)C=C2N1

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