Product Data Sheet

Product Name: Ensartinib (X-396)
Cat. No.: GC33190

Chemical Properties

Cas. No.	1370651-20-9		
SMILES	O=C(C1=NN=C(N)C(O[C@@H](C2=C(Cl)C=CC(F)=C2Cl)C)=C1)NC3=CC=C(C(N4C[C@@H](C)N[C@@H](C)C4)=O)C=C3		
Formula	$C_{26}H_{27}Cl_2FN_6O_3$	M.Wt	561.44
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	Ensartinib (X-396)		

Protocol

Cell experiment:

For viability experiments, cells are seeded in 96-well plates at 25%-33% confluency and exposed to drugs.The human lung adenocarcinoma cell lines H3122 and H2228 are treated with Ensartinib (10, 30, 100, 300 and 1000 nM). SUDHL-1 lymphoma cells are treated with Ensartinib (5, 10, 30, 100 and 300 nM). SY5Y neuroblastoma cells are treated with Ensartinib (30, 100, 300 and 1000 nM). At 72 hours post Ensartinib addition, Cell Titer Blue Reagent is added and fluorescence is measured on a Spectramax spectrophotometer. All experimental points are set up in hextuplicate replicates and are performed at least two independent times. IC50s are calculated using GraphPad Prism version 5 for Windows. The curves are fit using a nonlinear regression model with a log (inhibitor) vs. response formula[1].

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Animal experiment:

Mice[1] Nude mice (nu/nu) are injected with H3122 cells. Once tumors reach an average volume of 450 mm3, a total of 27 athymic mice harboring H3122 tumors are randomized and dosed via oral gavage with 25mg/kg Ensartinib (X-396) or the control vehicle. Two, five, and fifteen hours after the single treatment (3 tumors/timepoint/group), mice are sacrificed and serum is collected for assessment of drug concentration using an LC-MS based bioanalytical method.

References:

[1]. Lovly CM, et al. Insights into ALK-driven cancers revealed through development of novel ALK tyrosine kinaseinhibitors. Cancer Res. 2011 Jul 15;71(14):4920-31.

Background

Ensartinib is a potent and selective inhibitor of anaplastic lymphoma kinase (ALK; IC_{50} < 0.4 nM in a KINOMEscan kinase activity assay).[1] It reduces ALK autophosphorylation and inhibits endogenous ALK phosphorylation and activation of downstream targets ERK and Akt in H3122 cells. Ensartinib reduces growth of H3122 lung cancer cells harboring gain-of-function ALK-fusion proteins (IC_{50} = 15 nM) but has no effect on cell growth driven by other mutant kinases or that of non-cancerous HepG2 cells. Ensartinib, at a dose of 25

mg/kg, reduces H3122 xenograft growth with no effect on body weight in nude mice. It is also brain-permeable to a concentration of 65 nM.

1.Lovly, C.M., Heuckmann, J.M., de Stanchina, E., et al.Insights into ALK-driven cancers revealed through development of novel ALK tyrosine kinase inhibitorsCancer Res.71(14)4920-4931(2011)

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