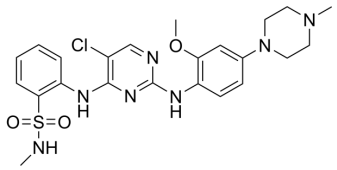
ALK inhibitor 2

Cat. No.:	HY-15358
CAS No.:	761438-38-4
Molecular Formula:	$C_{23}H_{28}ClN_7O_3S$
Molecular Weight:	518.03
Target:	Anaplastic lymphoma kinase (ALK); FAK
Pathway:	Protein Tyrosine Kinase/RTK
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (96.52 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9304 mL	9.6519 mL	19.3039 mL
	5 mM	0.3861 mL	1.9304 mL	3.8608 mL
	10 mM	0.1930 mL	0.9652 mL	1.9304 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (4.83 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.83 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ALK inhibitor 2 (compound 18) is a potent pyrimidin ALK inhibitor. ALK inhibitor 2 is a potent inhibitor of testis-specific serine/threonine kinase 2 (TSSK2; IC_{50}=37 nM) and focal adhesion kinase (FAK; IC_{50}=5 nM)[1].

IC_{50} & Target

IC50: 37 nM (TSSK2) and 5 nM (FAK)[1]

In Vitro

Testis-specific serine/threonine kinase 2 (TSSK2) is an important target for reversible male contraception. ALK inhibitor 2 (compound 18) contains a methylpiperazine A ring (R1=Me, X=N) and a D ring with R5=methylsulfonamide. ALK inhibitor 2 can undergo metabolic oxidation to form reactive adducts in the presence of glutathione[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Jon E Hawkinson, et al. Potent Pyrimidine and Pyrrolopyrimidine Inhibitors of Testis-Specific Serine/Threonine Kinase 2 (TSSK2). ChemMedChem. 2017 Nov 22;12(22):1857-1865.

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