ERK5-IN-2

Cat. No.: HY-128341

CAS No.: 1888305-96-1

Molecular Formula: $C_{17}H_{11}BrFN_3O_2$

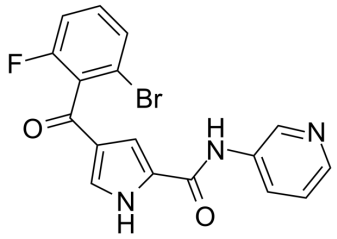
Molecular Weight: 388.19

Target: ERK

Pathway: MAPK/ERK Pathway; Stem Cell/Wnt

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (644.01 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5761 mL	12.8803 mL	25.7606 mL
	5 mM	0.5152 mL	2.5761 mL	5.1521 mL
	10 mM	0.2576 mL	1.2880 mL	2.5761 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: ≥ 2.08 mg/mL (5.36 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.36 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.36 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ERK5-IN-2 is an orally active, sub-micromolar, selective ERK5 inhibitor with IC_{50}s of 0.82 μM, 3 μM for ERK5 and ERK5 MEF2D, respectively. ERK5-IN-2 does not interact with the BRD4 bromodomain. ERK5-IN-2 suppresses both tumor xenograft growth and basic fibroblast growth factor (bFGF) driven Matrigel plug angiogenesis[1].

IC_{50} & Target

ERK5	ERK5 MEF2D
0.82 μM (IC_{50})	3 μM (IC_{50})

In Vivo

ERK5-IN-2 (compound 46) (p.o.; 100 mg/kg; CD1 mice for 7 days and CD1 nude (nu/nu) mice for 10 days) has an anti-angiogenic effect and low concentrations of haemoglobin[1].

ERK5-IN-2 (i.v. or p.o.; 10 mg/kg for 0.083-24 hours) exhibits low intrinsic clearance and has high flux and a low efflux ratio (ER) in a caco-2 cell permeability assay in both human and mouse[1].

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

Animal Model:	Female CD1 mice (8-10 weeks old) with Matrigel inoculation and female CD1 nude (nu/nu) mice (8-10 weeks old) bearing A2780 human ovarian carcinoma xenografts[1]
Dosage:	100 mg/kg
Administration:	P.o.; twice-daily; CD1 mice for 7 days and CD1 nude (nu/nu) mice for 10 days
Result:	Tumor volumes were significantly reduced.

Animal Model:	Female CD1 mice at 8-10 weeks of age[1]
Dosage:	10 mg/kg
Administration:	I.v. or p.o.; 0.083-24 hours
Result:	The terminal plasma half-life was 38 min, with a plasma clearance of 27 mL/min/kg, and oral bioavailability of 68%.

REFERENCES

[1]. Myers SM, et al. Identification of a novel orally bioavailable ERK5 inhibitor with selectivity over p38α and BRD4. Eur J Med Chem. 2019 May 25;178:530-543.

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