Ulixertinib hydrochloride

Cat. No.: HY-15816A

CAS No.: 1956366-10-1

Molecular Formula: $C_{21}H_{23}Cl_3N_4O_2$

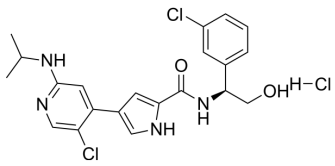
Molecular Weight: 469.79

Target: ERK

Pathway: MAPK/ERK Pathway; Stem Cell/Wnt

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 2 years; -20°C, 1 year (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (212.86 mM; Need ultrasonic)

H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.1286 mL	10.6431 mL	21.2861 mL
5 mM	0.4257 mL	2.1286 mL	4.2572 mL
10 mM	0.2129 mL	1.0643 mL	2.1286 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 (4.43 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.43 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.43 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Ulixertinib hydrochloride (BVD-523 hydrochloride) is a potent, orally active, highly selective, ATP-competitive and reversible covalent inhibitor of ERK1/2 kinases, with an IC_{50} of <0.3 nM against ERK2. Ulixertinib hydrochloride inhibits the phosphorylated ERK2 (pERK) and downstream kinase RSK (pRSK) in an A375 melanoma cell line[1][2].

In Vitro

Combined Ulixertinib (BVD-523; 10, 20, 30 μM; 48 hours) and VS-5584 treatment causes significant induction of cell death in human pancreatic cancer (HPAC) cells in PDAC cell lines BxPC-3, MIAPaCa-2, and CFPAC-1[3].

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

CUSTOMER VALIDATION

- Sci Transl Med. 2021 Jan 27;13(578):eaba7308.
- Nat Commun. 2023 Nov 2;14(1):6997.
- Nat Commun. 2023 May 19;14(1):2859.
- Nat Commun. 2022 Jul 14;13(1):4078.
- Adv Sci (Weinh). 2022 Oct;9(30):e2200717.

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REFERENCES

[1]. Ward RA, et al. Structure-Guided Design of Highly Selective and Potent Covalent Inhibitors of ERK1/2. J Med Chem. 2015 Jun 11;58(11):4790-801.

[2]. Changwen Ning, et al. Targeting ERK Enhances the Cytotoxic Effect of the Novel PI3K and mTOR Dual Inhibitor VS-5584 in Preclinical Models of Pancreatic Cancer. Oncotarget. 2017 Jul 4;8(27):44295-44311.

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