Balixafortide TFA

Cat. No.: HY-P1682A

Molecular Formula: $C_{86}H_{119}F_3N_{24}O_{23}S_2$

Molecular Weight: 1978.16

Sequence: Cyclo(Ala-Cys-Ser-Ala-{D-Pro}-{Dab}-Arg-Tyr-Cys-Tyr-Gln-Lys-{D-Pro}-Pro-Tyr-His) (Disulfide bridge: Cys2-Cys9)

Cyclo(ACSA-{D-Pro}-{Dab}-RYCYQK-{D-Pro}-PYH) (Disulfide bridge: Cys_2-Cys_9) (TFA)

Sequence Shortening: Cyclo(ACSA-{D-Pro}-{Dab}-RYCYQK-{D-Pro}-PYH) (Disulfide bridge: Cys2-Cys9)

Target: CXCR; Arrestin

Pathway: GPCR/G Protein; Immunology/Inflammation

Storage: Sealed storage, away from moisture and light

Powder -80°C 2 years

-20°C 1 year

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)

SOLVENT & SOLUBILITY

In Vitro

H_2O : 100 mg/mL (50.55 mM; Need ultrasonic)

DMSO : 100 mg/mL (50.55 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	0.5055 mL	2.5276 mL	5.0552 mL
5 mM	0.1011 mL	0.5055 mL	1.0110 mL
10 mM	0.0506 mL	0.2528 mL	0.5055 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 (1.26 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (1.26 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (1.26 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Balixafortide TFA (POL6326 TFA) is a potent, selective, well-tolerated peptidic CXCR4 antagonist with an IC_{50} < 10 nM. Balixafortide TFA shows 1000-fold selective for CXCR4 than a large panel of receptors including CXCR7. Balixafortide TFA blocks β-arrestin recruitment and calcium flux with IC_{50}s < 10 nM. Balixafortide TFA is also a potent hematopoietic stem and

	progenitor cell (HSPC) mobilizing agent. Anti-cancer effects[1][2].
IC_{50} & Target	CXCR4 <10 nM (IC_{50})
In Vitro	Balixafortide potently inhibits pERK / pAKT signaling in the lymphoma lines Namalwa (IC_{50}< 200 nM) and Jurkat (IC_{50} < 400 nM). Balixafortide efficiently blocks SDF-1 dependent chemotaxis of MDA MB 231 breast cancer cells (IC_{50} < 20 nM), Namalwa and Jurkat cells (IC_{50} < 10 nM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Balixafortide is optimized for favorable mouse absorption, distribution, metabolism and excretion (ADME) properties with balanced plasma protein binding, greater plasma and microsomal stability[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Zimmermann J, et al. Anti-tumor cell activity and in vitro profile of the next generation CXCR4 antagonist Balixafortide. Ann Oncol. 2018 Oct;29 Suppl 8:viii103.

[2]. Karpova D, et al. Mobilization of hematopoietic stem cells with the novel CXCR4 antagonist POL6326 (balixafortide) in healthy volunteers-results of a dose escalation trial. J Transl Med. 2017 Jan 3;15(1):2.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA