BIO5192 hydrate

Cat. No.: HY-107589A

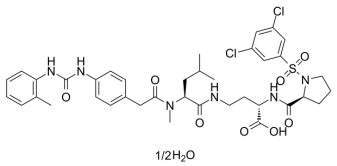
Molecular Formula: $C_{38}H_{46}Cl_2N_6O_8S.1/2H_2O$

Molecular Weight: 826.79

Target: Integrin

Pathway: Cytoskeleton

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



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (120.95 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.2095 mL	6.0475 mL	12.0950 mL
5 mM	0.2419 mL	1.2095 mL	2.4190 mL
10 mM	0.1209 mL	0.6047 mL	1.2095 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 (3.02 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.02 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BIO5192 hydrate is a selective and potent integrin α4β1 (VLA-4) inhibitor (K_d<10 pM). BIO5192 hydrate selectively binds to α4β1 (IC_{50}=1.8 nM) over a range of other integrins. BIO5192 hydrate results in a 30-fold increase in mobilization of murine hematopoietic stem and progenitors (HSPCs) over basal levels[1][2].

IC_{50} & Target

α4β1	α9β1	α2β1	α4β7
1.8 nM (IC_{50})	138 nM (IC_{50})	1053 nM (IC_{50})	>500 nM (IC_{50})

In Vivo

The combination of BIO5192 hydrate (1 mg/kg; i.v.) and Plerixafor (5 mg/kg; s.c.) exert an additive effect on progenitor mobilization[1].
BIO5192 hydrate (30 mg/kg; s.c; bid; during days 5 through 14) delays paralysis associated with EAE (experimental

autoimmune encephalomyelitis)[2].

BIO5192 hydrate (1 mg/kg, i.v.) shows the terminal half-life is 1.1 hours. BIO5192 hydrate (3, 10, and 30 mg/kg; s.c.) shows half-lives of 1.7, 2.7, and 4.7 hours, respectively. The blood plasma curves show that the AUC for the s.c. route of administration increased about 2.5-fold from 5,460 h*ng/ml for the 3 mg/kg dose to 14,175 h*ng/ml for the 30 mg/kg[1].

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

Animal Model:	C57BL/6J x 129Sv/J F1 mice[1]
Dosage:	1 mg/kg (with Plerixafor: 5 mg/kg)
Administration:	I.v.
Result:	Exerted an additive effect on progenitor mobilization.

Animal Model:	Healthy female Lewis rats weighing 150g[2]
Dosage:	30 mg/kg
Administration:	S.c; bid; during days 5 through 14
Result:	Showed a 3-day delay in onset of disease.

REFERENCES

[1]. Ramirez P, et al. BIO5192, a small molecule inhibitor of VLA-4, mobilizes hematopoietic stem and progenitor cells. Blood. 2009;114(7):1340-1343.

[2]. Leone DR, et al. An assessment of the mechanistic differences between two integrin alpha 4 beta 1 inhibitors, the monoclonal antibody TA-2 and the small molecule BIO5192, in rat experimental autoimmune encephalomyelitis. J Pharmacol Exp Ther. 2003;305(3):

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