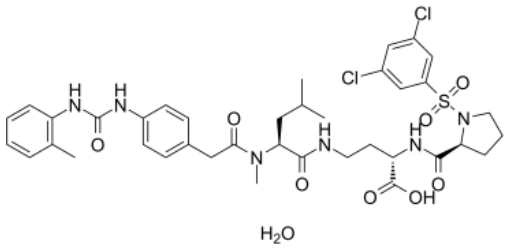
Product Data Sheet

Product Name: BIO5192 hydrate
Cat. No.: GC60077

Chemical Properties

Cas. No.			
SMILES	O=[S](N(CCC1)[C@@H]1C(N[C@H](C(O)=O)CCNC([C@H](CC(C)C)N(C)C(CC(C=C2)=CC=C2NC(NC(C=CC=C3)=C3C)=O)=O)=O)=O)(C4=CC(Cl)=CC(Cl)=C4)=O.O		
Formula	$C_{38}H_{46}Cl_2N_6O_8S.1/2H_2O$	M.Wt	826.79
Solubility		Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure			



Background

BIO5192 hydrate is a selective and potent integrin α4β1 (VLA-4) inhibitor (Kd<10 pM). BIO5192 hydrate selectively binds to α4β1 (IC50=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].

The combination of BIO5192 hydrate (1 mg/kg; i.v.) and Plerixafor (5 mg/kg; s.c.) exert an additive

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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]. Animal Model: C57BL/6J x 129Sv/J F1 mice[1]

[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):1150-1162.

Caution: Product has not been fully validated for medical applications. For research use only.
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