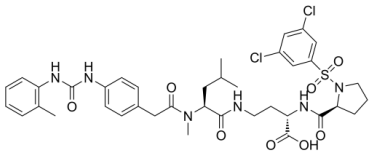
Data Sheet

Product Name:	BIO5192
Cat. No.:	CS-0028918
CAS No.:	327613-57-0
Molecular Formula:	$C_{38}H_{46}Cl_2N_6O_8S$
Molecular Weight:	817.78
Target:	Integrin
Pathway:	Cytoskeleton
Solubility:	DMSO : 12.5 mg/mL (15.29 mM; ultrasonic and warming and heat to 60°C)



BIOLOGICAL ACTIVITY:

BIO5192 is a selective and potent integrin **α4β1** (VLA-4) inhibitor (**K_d**<10 pM). BIO5192 selectively binds to α4β1 (**IC_{50}**=1.8 nM) over a range of other integrins. BIO5192 results in a 30-fold increase in mobilization of murine hematopoietic stem and progenitors (HSPCs) over basal levels[1][2]. ***In Vivo:*** The combination of BIO5192 (1 mg/kg; i.v.) and Plerixafor (5 mg/kg; s.c.) exert an additive effect on progenitor mobilization[1].

BIO5192 (30 mg/kg; s.c; bid; during days 5 through 14) delays paralysis associated with EAE (experimental autoimmune encephalomyelitis)[2].

BIO5192 (1 mg/kg, i.v.) shows the terminal half-life is 1.1 hours. BIO5192 (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].

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):1150–1162.

CAIndexNames:

Butanoic acid, 2-[[[(2S)-1-[(3,5-dichlorophenyl)sulfonyl]-2-pyrrolidinyl]carbonyl]amino]-4-[[(2S)-4-methyl-2-[methyl[2-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]amino]-1-oxopentyl]amino]-, (2S)-

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

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

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