Product Data Sheet

Product Name: PD-1/PD-L1 Inhibitor 3
Cat. No.: GC16258

Chemical Properties

Cas. No.	1629654-95-0
Chemical Name	(3S,6S,12S,15S,18S,21S,24S,27S,30R,39S,42S,47aS)-3-((1H-imidazol-5-yl)methyl)-12,18-bis((1H-indol-3-yl)methyl)-N,42-bis(2-amino-2-oxoethyl)-36-benzyl-21,24-dibutyl-27-(3-guanidinopropyl)-15-(hydroxymethyl)-6-isobutyl-8,20,23,38,39-pentamethyl-1,4,7,10,13,
SMILES	O=C(NCC(N)=O)[C@H]1NC([C@@H](NC([C@@H](N(C)C([C@H](CCCC)N(C)C([C@H](CC2=CNC3=C2C=CC=C3)NC([C@H](CO)NC([C@H](CC4=CNC5=C4C=CC=C5)NC(CN(C)C([C@H](CC(C)C)NC([C@@H](NC([C@H]6N(C([C@H](CC(N)=O)NC([C@@H](N(C(C(NC(CSC1)=O)CC7=CC=CC=C7)=O)C)C)=O)=O)CCC6)=O)CC8=CN=
Formula	$C_{89}H_{126}N_{24}O_{18}S$	M.Wt	1852.17
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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	PD-1/PD-L1 Inhibitor 3		

Background

PD-1/PD-L1 Inhibitor 3 is a PD-1/PD-L1 interaction inhibitor.

The anti-PD-1 and anti-PD-L1 compounds have been found to show impressive antitumor effects in various malignancies, such as melanoma. The greatest clinical outcome in unselected patients has been observed in melanoma. The tumor expression of PD-L1 is suggested to be a suggestive, inadequate, and predictive of response to immune-checkpoint blockade.

In vitro: PD-1/PD-L1 inhibitor 3 has been identified to be a potent and selective small

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molecule inhibitor blocking the interaction of programmed cell death protein 1 (PD-1) with its ligand protein (PD-L1) and with CD80. PD-1/PD-L1 inhibitor 3 was also found to act as an immunomodulator. In addition, PD-1/PD-L1 Inhibitor 3 was found to have highly efficacious binding to PD-L1 and promote the increased functional activities of T cells. Therefore, PD-1/PD-L1 inhibitor 3 could be regarded as a promising therapeutic treatment of cancer and infectious diseases, such as hepatitis C [1].

In vivo: So far, there is no animal in vivo study reported for PD-1/PD-L1 Inhibitor 3.

Clinical trial: Up to now, PD-1/PD-L1 Inhibitor 3 is still in the preclinical development stage.

References:
[1] MILLER Michael Matthew, et al. Patent, Pub. No.:WO/2014/151634