Product Datasheet

Technical Data

Formula	$C_{23}H_{25}ClN_2O_4S$					
Molecular Weight	460.97	**CAS No.**	854107-55-4			
Solubility (25°C)*	In vitro	DMSO	92 mg/mL (199.57 mM)			
		Ethanol	92 mg/mL (199.57 mM)			
		Water	Insoluble			
	In vivo (Add solvents to the product individually and in order)	Oral Administration	Homogeneous suspension	CMC-NA	≥5mg/ml	Taking the 1 mL working solution as an example, add 5 mg of this product to 1 ml of CMC-Na solution, mix evenly to obtain a homogeneous suspension with a final concentration of 5 mg/ml.
		Injection	Clear solution	5%DMSO [1]→ 40%PEG300 [2]→ 5%Tween80 [3]→ 50%ddH2O Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	4.6mg/ml (9.98mM)	Taking the 1 mL working solution as an example, add 50 μL of 92 mg/ml clarified DMSO stock solution to 400 μL of PEG300, mix evenly to clarify it; add 50 μL of Tween80 to the above system, mix evenly to clarify; then continue to add 500 μL of ddH2O to adjust the volume to 1 mL. The mixed solution should be used immediately for optimal results.
			Clear solution	5% DMSO [1]→ 95% Corn oil Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	0.65mg/ml (1.41mM)	Taking the 1 mL working solution as an example, add 50 μL of 13 mg/ml clear DMSO stock solution to 950 μL of corn oil and mix evenly. The mixed solution should be used immediately for optimal results.

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Capsid Bio tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.
* Room temperature shipping (Stability testing shows this product can be shipped at 2-8°C for storage purposes.)

Preparing Stock Solutions

Concentration \ Volume \ Mass	1 mg	5 mg	10 mg
1 mM	2.1693 mL	10.8467 mL	21.6934 mL
5 mM	0.4339 mL	2.1693 mL	4.3387 mL
10 mM	0.2169 mL	1.0847 mL	2.1693 mL
50 mM	0.0434 mL	0.2169 mL	0.4339 mL

Biological Activity

Description	Ponesimod (ACT-128800) is an orally active, selective **sphingosine-1-phosphate receptor 1 (S1P1)** immunomodulator with EC50 of 5.7 nM.
Targets	S1P1 receptor [1] (In recombinant Chinese hamster ovary cells) 5.7 nM(EC50)
In vitro	Relative to the potency of S1P, the potency of ponesimod at human recombinant receptors was 4.4-fold higher for S1P1 and 150-fold lower for human S1P3. Therefore, this compound was ~650-fold more selective for human S1P1 over S1P3 than the natural ligand[1].
In vivo	Ponesimod is a new, potent, and selective S1P1 receptor agonist with pharmacokinetic properties allowing rapid restoration of lymphocyte count in peripheral blood upon discontinuation. This compound prevents edema formation, inflammatory cell accumulation, and cytokine release in the skin of mice with delayed-type hypersensitivity. It also prevents the increase in paw volume and joint inflammation in rats with adjuvant-induced arthritis. Selective activation of S1P1 using this compound leads to blood lymphocyte count reduction and prevention in models of lymphocyte-mediated tissue inflammation. It has the potential to be as effective in animal models of autoimmunity and human autoimmune disease via its effect on T and B cell blood count. Thus, this compound may represent a new therapeutic option for the treatment of autoimmune diseases[1]. This chemical is eliminated within 1 week of discontinuation and its pharmacological effects are rapidly reversible [2].

Protocol (from reference)

Kinase Assay:[1]

- **GTPγS Binding Assay**
  GTPγS binding assays use membrane preparations of cells expressing recombinant S1P receptors of human, rat, or mouse origin. EC50 values were determined using IC50 Witch. Results were expressed as EC50 using the maximal response generated by S1P (percentage effect of maximal response) as an external maximum and solvent as minimum. Data are expressed as nanomoles of EC50 (geometric mean, geometric standard deviation).

Animal Study:[1]

- **Animal Models**
  Male Wistar rats; Female BALB/c mice
- **Dosages**
  5 to 10 ml/kg(Rats); 5 ml/kg(Mice)
- **Administration**
  Oral administration

References

https://pubmed.ncbi.nlm.nih.gov/21345969/ https://pubmed.ncbi.nlm.nih.gov/26770667/ https://pubmed.ncbi.nlm.nih.gov/21345969/

RETURN POLICY

Capsid Bio's Unconditional Return Policy ensures a smooth online shopping experience for our customers. If you are in any way unsatisfied with your purchase, you may return any item(s) within 7 days of receiving it. In the event of product quality issues, either protocol related or product related problems, you may return any item(s) within 365 days from the original purchase date. Please follow the instructions below when returning products.

SHIPPING & STORAGE

Capsid Bio products are transported at room temperature. If you receive the product at room temperature, please rest assured, the Capsid Bio Quality Inspection Department has conducted experiments to verify that the normal temperature placement of one month will not affect the biological activity of powder products. After collecting, please store the product according to the requirements described in the datasheet. Most Capsid Bio products are stable under the recommended conditions.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

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