

GBT1118

Chemical Properties

CAS No. : 1628799-51-8

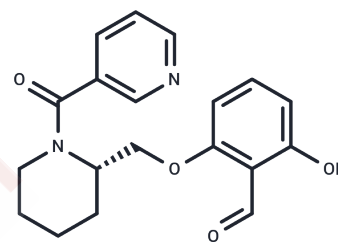
Formula: C₁₉H₂₀N₂O₄

Molecular Weight: 340.37

Store at low temperature

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



Biological Description

Description	GBT1118 is an orally active allosteric modulator of haemoglobin oxygen affinity, enhancing tolerance to acute severe hypoxia and suitable for hypoxia research.
Targets(IC50)	Reactive Oxygen Species
In vitro	GBT1118 forms a covalent and reversible bond with the N-terminal valine of the alpha chain of hemoglobin through an imine intermediate, allosterically enhancing the affinity of intracellular hemoglobin for O ₂ [1]. At concentrations equivalent to 25% of sample hemoglobin, GBT1118 can protect red blood cells from damage during severe hypoxia [2].
In vivo	GBT1118, at dosages of 70 or 140 mg/kg administered orally once, enhanced the tolerance of mice to severe hypoxemia [1]. In pharmacokinetic analyses, male mice receiving 10 mg/kg intravenously showed a blood half-life of 13.9 hours and plasma half-life of 11.3 hours, with blood and plasma area under the curve (AUC) at 2929 µg·h/mL and 60 µg·h/mL respectively. The steady state volume of distribution (V _{ss}) and systemic clearance (CL _s) in blood were 0.07 L/kg and 0.06 mL/min/kg, with a blood/plasma ratio of 51.4. Following 100 mg/kg orally, the time to reach maximum concentration (T _{max}) in blood was 2 hours with a peak concentration (C _{max}) of 318 µg/mL, while in plasma, T _{max} was 8 hours with a C _{max} of 12 µg/mL. The AUC was 13428 µg·h/mL in blood and 224 µg·h/mL in plasma, and bioavailability (F%) was found to be 45.8% and 33.5% respectively. In an acute hypoxia model with C57Bl/6 mice, a single oral dose improved their tolerance to a 5% O ₂ environment, facilitated greater oxygen delivery during hypoxic conditions maintaining mean arterial pressure (MAP), heart rate (HR), blood flow, and aerobic metabolism, and increased oxygen saturation in lung blood. This also led to reduced hypoxemia in vital tissues and decreased lactate levels [1].

Solubility Information

Solubility	DMSO: 80 mg/mL (235.04 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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A DRUG SCREENING EXPERT

In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 3.3 mg/mL (9.7 mM),Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.938 mL	14.6899 mL	29.3798 mL
5 mM	0.5876 mL	2.938 mL	5.876 mL
10 mM	0.2938 mL	1.469 mL	2.938 mL
50 mM	0.0588 mL	0.2938 mL	0.5876 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Dufu K, et al. GBT1118, a potent allosteric modifier of hemoglobin O2 affinity, increases tolerance to severe hypoxia in mice. *Am J Physiol Heart Circ Physiol.* 2017 Aug 1;313(2):H381-H391.

Tarasev M, et al. GBT1118, a voxelotor analog, protects red blood cells from damage during severe hypoxia. *Am J Transl Res.* 2022 Jan 15;14(1):240-251.

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