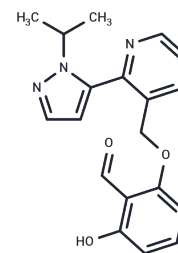


voxelotor

Chemical Properties

CAS No. :	1446321-46-5
Formula:	C ₁₉ H ₁₉ N ₃ O ₃
Molecular Weight:	337.37
Storage:	Store at low temperature Powder: -20°C for 3 years In solvent: -80°C for 1 year <i>Actual storage temperature shall be subject to the COA.</i>



Biological Description

Description	Voxelotor (GBT 440) is a novel hemoglobin S (HbS) polymerization inhibitor primarily used for the treatment of sickle cell disease (SCD) and a cytochrome P450 3A4 inhibitor. Voxelotor targets and covalently binds to the N-terminal valine of the HbS alpha chain, thereby stabilizing sickle cell hemoglobin (HbS).
Targets(IC50)	Others
In vitro	<p>METHODS: Voxelotor (3-30 μmol/L) was incubated with hemoglobin (25 μmol/L) in TES or saline buffer at 37 °C for 45 min, and changes in the binding affinity of O₂ for Hb were measured using a TCS hematology analyzer.</p> <p>RESULTS: Voxelotor, a small molecule that binds to the N-terminal α-chain of Hb, increases the affinity of HbS for oxygen, delays HbS polymerization in vitro and prevents erythrocyte sickling. [1]</p> <p>METHODS: HepG2 cells were treated with Voxelotor (1 μg/mL) and their metabolites were analyzed by liquid chromatography, high-resolution MS and tandem MS.</p> <p>RESULTS: Voxelotor can be used for the identification of phase I and phase II metabolites in vitro. [2]</p>
In vivo	<p>METHODS: To assess the activity and efficacy of Voxelotor, Voxelotor (100-150 mg/kg, 0.5% methylcellulose/0.5% SDS) was administered by gavage to a mouse model of SCD twice daily for 9-12 days.</p> <p>RESULTS: Voxelotor reduced isolated sickle cells and prolonged erythrocyte half-life in the SCD mouse model. [1]</p>

Solubility Information

Solubility	DMSO: 79 mg/mL (234.16 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (5.93 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>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.9641 mL	14.8205 mL	29.641 mL
5 mM	0.5928 mL	2.9641 mL	5.9282 mL
10 mM	0.2964 mL	1.4821 mL	2.9641 mL
50 mM	0.0593 mL	0.2964 mL	0.5928 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

- Oksenberg D, et al. GBT440 increases haemoglobin oxygen affinity, reduces sickling and prolongs RBC half-life in a murine model of sickle cell disease. *Br J Haematol.* 2016 Oct; 175(1):141-53.
- Shu P, You G, Li W, et al. Cefmetazole sodium as an allosteric effector that regulates the oxygen supply efficiency of adult hemoglobin. *Journal of Biomolecular Structure and Dynamics.* 2023: 1-15.
- Rzeppa S, et al. Identification of human in vitro metabolites of the haemoglobin S polymerization inhibitor voxelotor for doping control purposes. *Drug Test Anal.* 2023 Nov-Dec; 15(11-12):1403-1409.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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