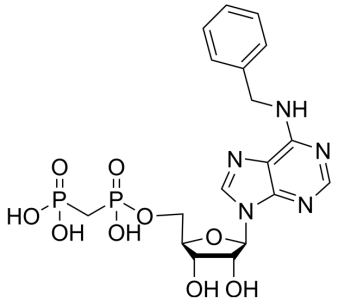
PSB-12379

Cat. No.:	HY-100747
CAS No.:	1802226-78-3
Molecular Formula:	$C_{18}H_{23}N_5O_9P_2$
Molecular Weight:	515.35
Target:	CD73
Pathway:	Immunology/Inflammation
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

H_2O : 125 mg/mL (242.55 mM; Need ultrasonic)
DMSO : ≥ 5 mg/mL (9.70 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.9404 mL	9.7021 mL	19.4043 mL
5 mM	0.3881 mL	1.9404 mL	3.8809 mL
10 mM	0.1940 mL	0.9702 mL	1.9404 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: PBS
Solubility: 100 mg/mL (194.04 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

PSB-12379, a nucleotide analogue, is a potent Ecto-5'-Nucleotidase (CD73) inhibitor with K_is of 9.03 nM (rat) and 2.21 nM (human)[1][2].

IC_{50} & Target

Ki: 9.03 nM (rat), 2.21 nM (human) (Ecto-5'-Nucleotidase)[1]

In Vitro

Metabolism: Only a small percentage (<23%) of PSB-12379 (10g) is metabolized under the applied conditions, while >77% of the compounds are recovered unchanged after a long incubation for 8 h. PSB-12379 (10g) is somewhat less stable, and 56% are metabolized within 8 h. Hydrolytic cleavage of the glycosidic bond, which is a typical phase I reaction of nucleosides and nucleotides, was observed as the main reaction[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Front Bioeng Biotechnol. 2022 Apr 27;10:895998.
- Cancers (Basel). 2022, 14(23), 5750
- SSRN. 2023 Jul 28.

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REFERENCES

[1]. Bhattarai S, et al. α,β-Methylene-ADP (AOPCP) Derivatives and Analogues: Development of Potent and Selective ecto-5'-Nucleotidase (CD73) Inhibitors. J Med Chem. 2015 Aug 13;58(15):6248-63.

[2]. X-Ray Co-Crystal Structure Guides the Way to Subnanomolar Competitive Ecto-5 -Nucleotidase (CD73) Inhibitors for Cancer Immunotherapy Sanjay Bhattarai. Adv. Therap. 2019, 2, 1900075.

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