

JBSNF-000028

## Chemical Properties

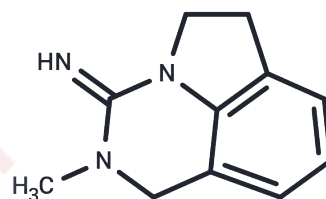
CAS No. :

Formula: C<sub>11</sub>H<sub>13</sub>N<sub>3</sub>

Molecular Weight: 187.24

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	JBSNF-000028 belongs to small molecule inhibitors, serving as a nicotinamide N-methyltransferase (NNMT) inhibitor (IC <sub>50</sub> =33 nM (human), 190 nM (monkey), 210 nM (mouse)), with oral activity and cell permeability, for research on metabolic disorders, possessing insulin-sensitizing, glucose-lowering, and weight-reducing effects.
Targets(IC <sub>50</sub> )	Others
In vitro	<b>Methods:</b> The inhibitory effect of JBSNF-000028 hydrochloride on NNMT activity was evaluated in U2OS cells (24 hours); cytotoxicity was detected in HepG2 cells (72 hours); and the binding mechanism and selectivity were studied through structural analysis and broad target screening. <b>Results:</b> JBSNF-000028 hydrochloride inhibited NNMT activity with an EC <sub>50</sub> of 2.5 μM; showed no cytotoxicity to HepG2 cells (10-100 μM); bound through a hairpin structure located beneath the nicotinamide pocket by stacking with Tyr-204 and Leu-164; and exhibited no activity against metabolism and safety-related target panels. [1]
In vivo	<b>Methods:</b> In diet-induced obese (DIO) mice and NNMT knockout DIO mice, JBSNF-000028 hydrochloride (50 mg/kg; twice daily) was administered orally for 27 days and 4 weeks, respectively, to evaluate its effects on glucose and lipid metabolism. <b>Results:</b> JBSNF-000028 hydrochloride improved glucose and lipid metabolism in DIO mice and enhanced glucose tolerance in NNMT knockout DIO mice. [1]

## Solubility Information

Solubility	DMSO: 8.8 mg/mL (47 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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### Preparing Stock Solutions

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	1mg	5mg	10mg
1 mM	5.3407 mL	26.7037 mL	53.4074 mL
5 mM	1.0681 mL	5.3407 mL	10.6815 mL
10 mM	0.5341 mL	2.6704 mL	5.3407 mL
50 mM	0.1068 mL	0.5341 mL	1.0681 mL

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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

Ruf S, et al. Novel tricyclic small molecule inhibitors of Nicotinamide N-methyltransferase for the treatment of metabolic disorders. Sci Rep. 2022 Sep 14;12(1):15440.

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Tel:781-999-4286 E\_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481