JBSNF-000028 TFA

Cat. No.: HY-151500A

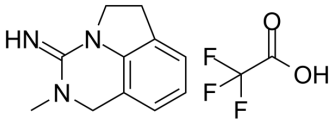
Molecular Formula: $C_{13}H_{14}F_3N_3O_2$

Molecular Weight: 301.26

Target: Others

Pathway: Others

Storage: 4°C, sealed storage, away from moisture and light
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (331.94 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.3194 mL	16.5970 mL	33.1939 mL
5 mM	0.6639 mL	3.3194 mL	6.6388 mL
10 mM	0.3319 mL	1.6597 mL	3.3194 mL

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

BIOLOGICAL ACTIVITY

Description

JBSNF-000028 TFA is an orally active nicotinamide N-methyltransferase (NNMT) inhibitor with IC_{50}s of 0.033 μM, 0.19 μM and 0.21 μM against human NNMT (hNNMT), monkey NNMT (mkNNMT), and mouse NNMT (mNNMT), respectively. JBSNF-000028 TFA can be used for the research of metabolic disorders[1].

IC_{50} & Target

IC_{50}: 0.033 μM (hNNMT), 0.19 μM (mkNNMT), 0.21 μM (mNNMT)[1]

In Vitro

JBSNF-000028 TFA (24 h) inhibits NNMT activity with an EC_{50} of 2.5 μM in U2OS cells[1].
JBSNF-000028 TFA (10-100 μM; 72 h) has no cytotoxicity against HepG2 cells[1].
JBSNF-000028 TFA binds below a hairpin structural motif at the nicotinamide pocket and stacks between Tyr-204 (from Hairpin) and Leu-164 (from central domain)[1].
JBSNF-000028 TFA is inactive against a broad panel of targets related to metabolism and safety[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

JBSNF-000028 TFA (50 mg/kg; p.o.; twice daily for 27 days) improves glucose and lipid handling in mice with diet-induced obesity (DIO)[1].
JBSNF-000028 TFA (50 mg/kg; p.o.; twice daily for 4 weeks) improves glucose tolerance in NNMT knockout mice with diet-

induced obesity[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. 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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