NNMT-IN-4

Cat. No.: HY-151813

CAS No.: 2947393-64-6

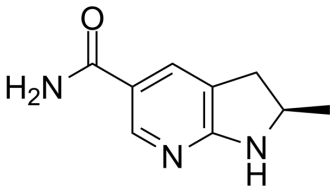
Molecular Formula: $C_9H_{11}N_3O$

Molecular Weight: 177.2

Target: Others

Pathway: Others

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

NNMT-IN-4 (compound 38) is a selective, uncompetitive and membrane permeability nicotinamide N-methyltransferase (NNMT) inhibitor with IC_{50} values of 42 and 38 nM in vitro biochemical and cell-based assays, respectively. NNMT-IN-4 shows favorable PK/PD and safety profiles as well as excellent oral bioavailability and pharmaceutical properties. NNMT-IN-4 can be used as a vivo chemical probe of NNMT[1].

IC_{50} & Target

IC50: 38 nM (NNMT, in K562 cells), 42 nM (promega MTase-Glo methyltransferase assay)[1]

In Vitro

NNMT-IN-4 (5 nM-0.5 mM; 24 h) shows inhibitory effect to NNMT with an IC_{50} value of 38 nM in K562 cells[1].

NNMT-IN-4 (5 nM-0.5 mM; 24 h) shows inhibitory effect to NNMT with an IC_{50} value of 42 nM in promega MTase-Glo methyltransferase assay[1].

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

In Vivo

Pharmacokinetic Properties of NNMT-IN-4 in Mice[1].

	Mice PO 50 mg/kg
$T_{1/2}$ (h)	2.89
T_{max} (h)	0.250
C_{max} (ng/mL)	22500
AUC_{last} (ng*h/mL)	51115
CI (1 mg/kg IV) (mL/min/kg)	36.1
F (%)	220

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

REFERENCES

[1]. Barrows RD, et al. Potent Uncompetitive Inhibitors of Nicotinamide N-Methyltransferase (NNMT) as In Vivo Chemical Probes. J Med Chem. 2022 Nov 10;65(21):14642-14654.

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