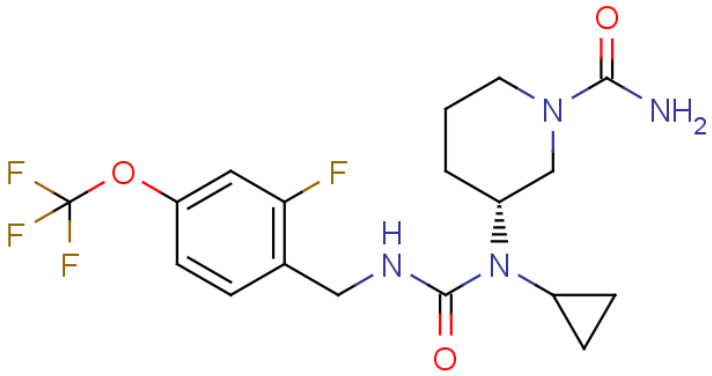
Name: JNT-517

Cat#: EX-A8059

Target: Amino acid Transporter
Pathway: Membrane Transporter/Ion Channel

Chemical Structure:



Chemical Name	1-Piperidinecarboxamide, 3-[cyclopropyl[[[[2-fluoro-4-(trifluoromethoxy)phenyl]methyl]amino]carbonyl]amino]-, (3R)-
Canonical SMILES	O=C(N)N1CCCC(N(C(=O)NCC2=CC=C(OC(F)(F)F)C=C2F)C3CC3)C1
InChI	InChI=1S/C18H22F4N4O3/c19-15-8-14(29-18(20,21)22)6-3-11(15)9-24-17(28)26(12-4-5-12)13-2-1-7-25(10-13)16(23)27/h3,6,8,12-13H,1-2,4-5,7,9-10H2,(H2,23,27)(H,24,28)/t13-/m1/s1
InChI Key	FNRHWODWSBDOOY-CYBMUJFWSA-N

Molecular Weight	418.3859	Storage	2 years -20°C powder 1 month -20°C in solvent
Formula	C18H22F4N4O3		
CAS No.	2837993-05-0	Synonyms	JNT 517; JNT517; Repinatrabit

Solubility (25°C) *	In vitro	DMSO	DMSO
		Ethanol	N/A
		Water	N/A
	In vivo (should be freshly prepared each time)		

* <1 mg/ml means slightly soluble or insoluble.

* Please note that Selleck tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.

Preparing Stock Solutions:

Mass / Volume / Concentration	1 mg	5 mg	10 mg
1 mM	2.3901 mL	11.9506 mL	23.9011 mL
5 mM	0.4780 mL	2.3901 mL	4.7802 mL
10 mM	0.2390 mL	1.1951 mL	2.3901 mL

DMSO : *The above data is based on the product molecular weight 418.389.

In Vivo	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ⩾ 5 mg/mL (11.95 mM); Clear solution 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ⩾ 5 mg/mL (11.95 mM); Clear solution 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ⩾ 5 mg/mL (11.95 mM); Clear solution

Biological Activities:

Description	JNT-517 is an orally active, selective SLC6A19 allosteric inhibitor with an IC50 of 47 nM for human SLC6A19. JNT-517 can be used for the study of phenylketonuria (PKU)[1].
IC_{50} & Target	SLC6A19[1]
In Vivo	JN-170 (precursor of JN-517) (50-250 mg/kg, po, single dose) increases the excretion of amino acids in urine in mouse models[2] .

References	[1]. Dean G Brown, et al. Small molecule inhibitors of mammalian slc6a19 function. Patent WO2022192370A1. [2]. Wobst HJ, et al., SLC6A19 inhibition facilitates urinary neutral amino acid excretion and lowers plasma phenylalanine. JCI Insight. 2024 Nov 8;9(21):e182876.