MS48107

Cat. No.: HY-134494

CAS No.: 2375070-79-2

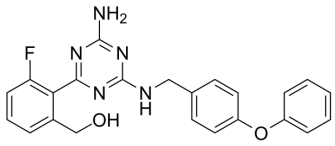
Molecular Formula: $C_{23}H_{20}FN_5O_2$

Molecular Weight: 417.44

Target: Others

Pathway: Others

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



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (239.56 mM; Need ultrasonic)

Preparing Stock Solutions	Concentration / Solvent / Mass	1 mg	5 mg	10 mg
	1 mM	2.3956 mL	11.9778 mL	23.9555 mL
	5 mM	0.4791 mL	2.3956 mL	4.7911 mL
	10 mM	0.2396 mL	1.1978 mL	2.3956 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (5.99 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.99 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

MS48107 is a potent and selective positive allosteric modulator of G protein-coupled receptor 68 (GPR68). MS48107 is selective for GPR68 over the closely related proton GPCRs, neurotransmitter transporters, and hERG ion channels. MS48107 can readily cross the blood-brain barrier (BBB) in mice[1].

In Vitro

5-HT2B has moderate binding affinity to MS48107 (compound 71) with a K_i value of 219 nM. At 5-HT2B receptors, MS48107 shows no agonist activity but display weak antagonist activity with a K_i value of 310 nM, respectively[1].
MS48107 (compound 71) has agonist activity only at the MT1 and MT2 receptors. MS48107 is a weak full agonist at the MT1 receptor (EC_{50} = 320 nM) and a weak partial agonist activity at the MT2 receptor (EC_{50} = 540 nM). MS48107 displays low binding affinities to MT1 (5900 nM) and MT2 (1100 nM) receptors[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo	For MS48107 (compound 71), a single intraperitoneal injection at the dose of 25 mg/kg leads to high exposure levels (above 10 μM) in both plasma and brain at 0.5 h in mice (Swiss Albino mice). The high compound exposure levels in both plasma and brain are maintained for 2 h[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Xufen Yu, et al. Design, Synthesis, and Characterization of Ogerin-Based Positive Allosteric Modulators for G Protein-Coupled Receptor 68 (GPR68). J Med Chem. 2019 Aug 22;62(16):7557-7574.

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