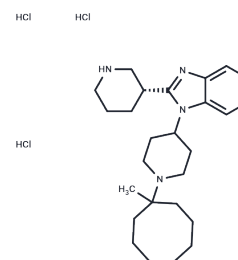


MCOPPB triHydrochloride

Chemical Properties

CAS No. :	1108147-88-1
Formula:	C ₂₆ H ₄₃ Cl ₃ N ₄
Molecular Weight:	518.01
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	MCOPPB triHydrochloride (MCOPPB 3HCl) is a nociceptin receptor agonist.
Targets(IC50)	Opioid Receptor
In vivo	Only Parthenolide, the HDAC inhibitor with anti-inflammatory features, displayed a potent anti-apoptotic effect in Phb1 KO hepatocytes. Indeed, TSA and Parthenolide-treated hepatocytes showed increased levels of FXR, and reduced levels of CYP7A1, HDAC4, TNF α , TRAIL and Bax suggesting a less toxic effect of bile acids as a results of specific HDAC inhibition, resulting in the attenuation of the Phb1 KO hepatocytes apoptotic response. Importantly, Parthenolide exerts a protective effect from the liver injury after BDL in Phb1 KO mice. Indeed, Parthenolide treatment results in a reduction of the mortality rate of this mice after BDL associated with a lower apoptotic response as revealed by a reduction of necrotic areas, Tunel-staining, as well as decreased ALT (8431 \pm 957 vs.4225 \pm 210 U/L) and AST (4805 \pm 300 vs.2242 \pm 438 U/L) activities compared to control Phb1 KO mice[3].
Kinase Assay	Binding assay: Kinases are produced displayed on T7 phage or by expression in HEK-293 cells and tagged with DNA. Binding reactions are performed at room temperature for 1 hour, and the fraction of kinase not bound to test compound is determined by capture with an immobilized affinity ligand and quantitation by quantitative PCR. Each kinase is tested individually against CEP-32496. Kd values are determined using eleven serial 3-fold dilutions and presented as mean values from experiments performed in duplicate. Variability between individual values is less than 2-fold.

Solubility Information

Solubility	DMSO: 32.04 mg/mL (61.85 mM),Sonication is recommended. H ₂ O: 16.02 mg/mL (30.93 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (3.86 mM),Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may</i>

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In vivo Formulation	<i>vary and should be modified based on specific experimental conditions.</i>
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9305 mL	9.6523 mL	19.3046 mL
5 mM	0.3861 mL	1.9305 mL	3.8609 mL
10 mM	0.193 mL	0.9652 mL	1.9305 mL
50 mM	0.0386 mL	0.193 mL	0.3861 mL

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

Hayashi, Shigeo; Hirao, Akiko; Imai, Aki; Nakamura, Hiroshi; Murata, Yoshinori; Ohashi, Katsuyo; Nakata, Eriko. Novel Non-Peptide Nociceptin/Orphanin FQ Receptor Agonist, 1-[1-(1-Methylcyclooctyl)-4-piperidiny]-2-[(3R)-3-piperidiny]-1H-benzimidazole: Design, Synthesis, and Structure-Activity Relationship of Oral Receptor Occupancy in the Brain for Orally Potent Antianxiety Drug. *Journal of Medicinal Chemistry* (2009), 52(3), 610-625.

Hayashi S, Hirao A, Imai A, Nakamura H, Murata Y, Ohashi K, Nakata E. Novel non-peptide nociceptin/orphanin FQ receptor agonist, 1-[1-(1-Methylcyclooctyl)-4-piperidiny]-2-[(3R)-3-piperidiny]-1H-benzimidazole: design, synthesis, and structure-activity relationship of oral receptor occupancy in the brain for orally potent antianxiety drug. *J Med Chem.* 2009 Feb 12;52(3):610-25.

Hirao A, Imai A, Sugie Y, Yamada Y, Hayashi S, Toide K. Pharmacological characterization of the newly synthesized nociceptin/orphanin FQ-receptor agonist 1-[1-(1-methylcyclooctyl)-4-piperidiny]-2-[(3R)-3-piperidiny]-1H-benzimidazole as an anxiolytic agent. *J Pharmacol Sci.* 2008 Mar;106(3):361-8. Epub 2008 Mar 5.

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