

JNJ-63533054

Chemical Properties

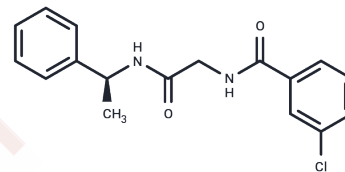
CAS No. : 1802326-66-4

Formula: C₁₇H₁₇ClN₂O₂

Molecular Weight: 316.78

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 | JNJ-63533054 is a potent and selective agonist of hGPR139 with an EC ₅₀ = 16 nM. |
| Targets(IC ₅₀) | GPCR |
| In vitro | JNJ-63533054 specifically activates human GPR139 in the calcium mobilization (EC ₅₀ = 16 ± 6 nM) and GTPγS binding (EC ₅₀ = 17 ± 4 nM) assays. JNJ-63533054 is found to be clean of any cross reactivity as judged by an external selectivity panel of 50 known GPCRs, ion channels, and transporters as well as our own internal whole cell lead generation biology selectivity panel. |
| In vivo | JNJ-63533054 is found to cross the blood-brain barrier and have good drug-like properties amenable for oral dosing in rat. JNJ-63533054 exhibits good stability in both human and rat microsomes and high solubility in aqueous media, and no DDI potential was found. JNJ-63533054 also activates the rat and mouse GPR139 receptor with similar potency (rat EC ₅₀ = 63 ± 24 nM, mouse EC ₅₀ = 28 ± 7 nM). |

Solubility Information

| | |
|---------------------|---|
| Solubility | DMSO: 45 mg/mL (142.05 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 (6.31 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 vary and should be modified based on specific experimental conditions.</i> |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|-------|-----------|------------|------------|
| 1 mM | 3.1568 mL | 15.7838 mL | 31.5676 mL |
| 5 mM | 0.6314 mL | 3.1568 mL | 6.3135 mL |
| 10 mM | 0.3157 mL | 1.5784 mL | 3.1568 mL |
| 50 mM | 0.0631 mL | 0.3157 mL | 0.6314 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

Dvorak CA, et al. ACS Med Chem Lett. 2015 Jul 20;6(9):1015-8.

Liu C, et al. Mol Pharmacol. 2015 Nov;88(5):911-25.

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