

hGPR91 antagonist 1

Chemical Properties

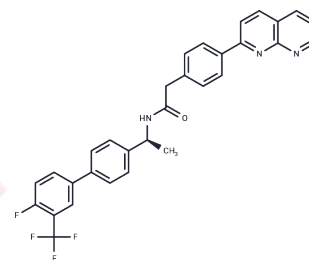
CAS No. : 1314796-00-3

Formula: C₃₁H₂₃F₄N₃O

Molecular Weight: 529.53

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	hGPR91 antagonist 1 is a potent and selective hGPR91 antagonist (IC ₅₀ : 7 nM).
Targets(IC ₅₀)	Succinate Receptor 1 (SUCNR1)
In vivo	GPR91, a 7TM G-Protein-Coupled Receptor, has been recently deorphanized with succinic acid as its endogenous ligand. Current literature indicates that GPR91 plays role in various pathophysiology including renal hypertension, autoimmune disease and retinal angiogenesis. Starting from a small molecule high-throughput screening hit 1 (hGPR91 IC ₅₀): 0.8 μM)-originally synthesized in Merck for Bradykinin B(1) Receptor (BK (1)R) program, systematic structure-activity relationship study led us to discover potent and selective hGPR91 antagonists e.g. 2c, 4c, and 5 g (IC ₅₀): 7-35 nM;>1000 fold selective against hGPR99, a closest related GPCR;>100 fold selective in Drug Matrix screening). Led to identification of two structurally distinct and orally bio-available lead compounds: 5g (%F: 26) and 7e (IC ₅₀): 180 nM;>100 fold selective against hGPR99;%F: 87).

Solubility Information

Solubility	DMSO: 37.5 mg/mL (70.82 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 3.75 mg/mL (7.08 mM), Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.75 mg/mL (7.08 mM), Solution. <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	1.8885 mL	9.4423 mL	18.8847 mL
5 mM	0.3777 mL	1.8885 mL	3.7769 mL
10 mM	0.1888 mL	0.9442 mL	1.8885 mL
50 mM	0.0378 mL	0.1888 mL	0.3777 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

Bhuniya D, et al. Discovery of a potent and selective small molecule hGPR91 antagonist. *Bioorg Med Chem Lett.* 2011 Jun 15;21(12):3596-602.

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