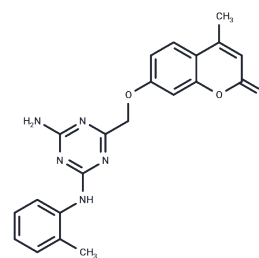


## GPR40/FFAR1 modulator 1

## Chemical Properties

CAS No. :	874755-26-7
Formula:	C <sub>21</sub> H <sub>19</sub> N <sub>5</sub> O <sub>3</sub>
Molecular Weight:	389.41
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	GPR40/FFAR1 modulator 1 is a Gq-coupled free fatty acid receptor 1 (GPR40/FFAR1) agonist and allosteric modulator.
Targets(IC50)	GPCR
In vitro	The long-chain fatty acid receptor FFAR1/GPR40 binds agonists in both an interhelical site between the extracellular segments of transmembrane helix (TM)-III and TM-IV and a lipid-exposed groove between the intracellular segments of these helices. Molecular dynamics simulations of FFAR1 with agonist removed demonstrated a major rearrangement of the polar and charged anchor point residues for the carboxylic acid moiety of the agonist in the interhelical site, which was associated with closure of a neighboring, solvent-exposed pocket between the extracellular poles of TM-I, TM-II, and TM-VII. A synthetic compound designed to bind in this pocket, and thereby prevent its closure, was identified through structure-based virtual screening and shown to function both as an agonist and as an allosteric modulator of receptor activation[1].

## Solubility Information

Solubility	DMSO: 30 mg/mL (77.04 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: 2 mg/mL (5.14 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

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	<b>1mg</b>	<b>5mg</b>	<b>10mg</b>
1 mM	2.568 mL	12.8399 mL	25.6799 mL
5 mM	0.5136 mL	2.568 mL	5.136 mL
10 mM	0.2568 mL	1.284 mL	2.568 mL
50 mM	0.0514 mL	0.2568 mL	0.5136 mL

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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

Lückmann M, et al. Molecular dynamics-guided discovery of an ago-allosteric modulator for GPR40/FFAR1. Proc Natl Acad Sci U S A. 2019 Apr 2;116(14):7123-7128.

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