

Product Name: AS2717638

Catalog No.: 7730

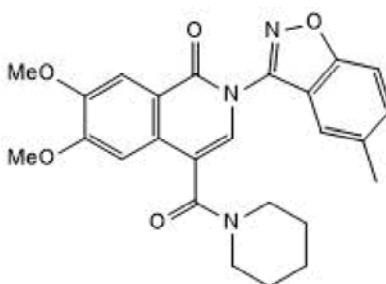
Batch No.: 1

CAS Number: 2148339-28-8

IUPAC Name: 6,7-Dimethoxy-2-(5-methyl-1,2-benzisoxazol-3-yl)-4-(1-piperidinylcarbonyl)-1(2*H*)-isoquinolinone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₅N₃O₅
Batch Molecular Weight: 447.48
Physical Appearance: Off-white solid
Solubility: DMSO to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.1	5.63	9.39
Found	66.69	5.55	9.18

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

AS2717638 is a potent LPA5 receptor antagonist ($IC_{50} = 38$ nM in BV-2 microglia cells). It is selective for LPA5 over LPA1, LPA2, and LPA3. It inhibits LPA-mediated pro-inflammatory transcription factor phosphorylation. *In vivo*, AS2717638 inhibits LPA5 agonist-induced allodynia in mice. It also exhibits analgesic effects against both neuropathic and inflammatory pain in rodent models. Orally bioavailable and brain penetrant.

Physical and Chemical Properties:

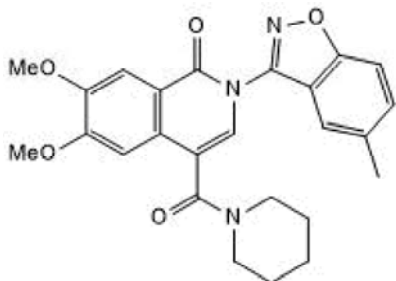
Batch Molecular Formula: $C_{25}H_{25}N_3O_5$

Batch Molecular Weight: 447.48

Physical Appearance: Off-white solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

DMSO to 10 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Joshi *et al* (2022) Lysophosphatidic acid receptor 5 (LPA5) knockout ameliorates the neuroinflammatory response *in vivo* and modifies the inflammatory and metabolic landscape of primary microglia *in vitro*. *Cells* **11** 1071. PMID: 35406635.

Joshi *et al* (2021) Inhibition of autotaxin and lysophosphatidic acid receptor 5 attenuates neuroinflammation in LPS-activated BV-2 microglia and a mouse endotoxemia model. *Int.J.Mol.Sci.* **22** 8519. PMID: 34445223.

Medeiros Geraldo *et al* (2021) Role of lysophosphatidic acid and its receptors in health and disease: novel therapeutic strategies. *Signal Transduct.Target.Ther.* **6** 45. PMID: 33526777.

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