

**Product Name:** ML 193

**Catalog No.:** 4860

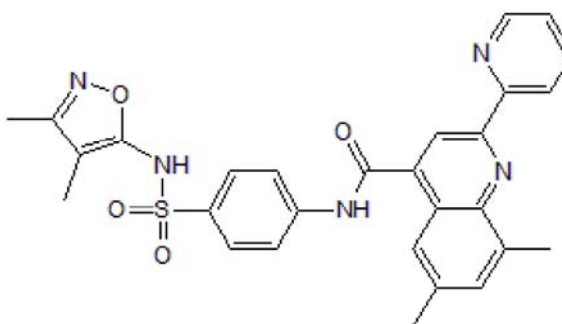
**Batch No.:** 2

CAS Number: 713121-80-3

IUPAC Name: *N*-[4-[[[3,4-Dimethyl-5-isoxazolyl)amino]sulfonyl]phenyl]-6,8-dimethyl-2-(2-pyridinyl)-4-quinolinecarboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>25</sub>N<sub>5</sub>O<sub>4</sub>S  
**Batch Molecular Weight:** 527.59  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	63.74	4.78	13.27
Found	63.54	4.68	13.07

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**Description:**

Selective GPR55 antagonist (IC<sub>50</sub> = 221 nM). Exhibits >27-, >145- and >145-fold selectivity for GPR55 over CB<sub>1</sub>, GPR35 and CB<sub>2</sub>, respectively. Inhibits ERK signaling in vitro.

**Physical and Chemical Properties:**

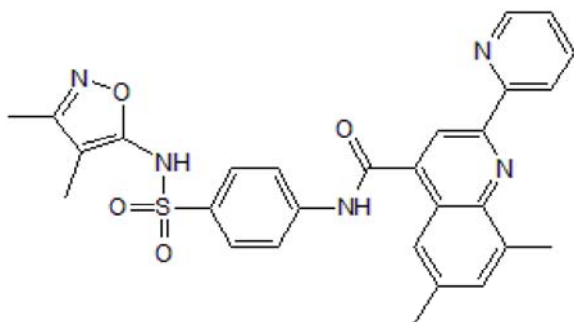
Batch Molecular Formula: C<sub>28</sub>H<sub>25</sub>N<sub>5</sub>O<sub>4</sub>S

Batch Molecular Weight: 527.59

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 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°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°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Kotsikorou *et al*** (2013) Identification of the GPR55 antagonist binding site using a novel set of high-potency GPR55 selective ligands. *Biochemistry* **52** 9456. PMID: 24274581.

**Heynen-Genel *et al*** (2010) Screening for selective ligands for GPR55 - antagonists. *Probe Reports from the NIH Molecular Libraries Program*. PMID: 22091481.

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