

Product Name: ML 193

Catalog No.: 4860

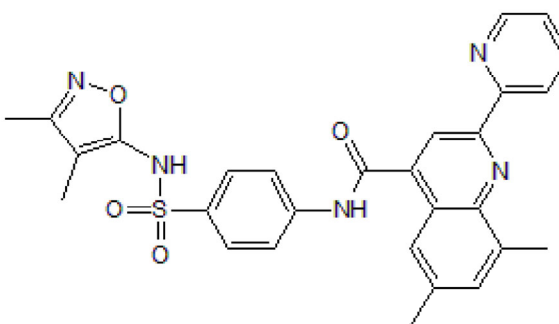
Batch No.: 3

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: C₂₈H₂₅N₅O₄S.
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 99.0% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.74	4.78	13.27
Found	62.78	4.72	13.09

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

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Description:

ML 193 is a selective GPR55 antagonist ($IC_{50} = 221$ nM). Exhibits >27-, >145- and >145-fold selectivity for GPR55 over CB₁, GPR35 and CB₂, respectively. Inhibits ERK signaling in vitro.

Physical and Chemical Properties:

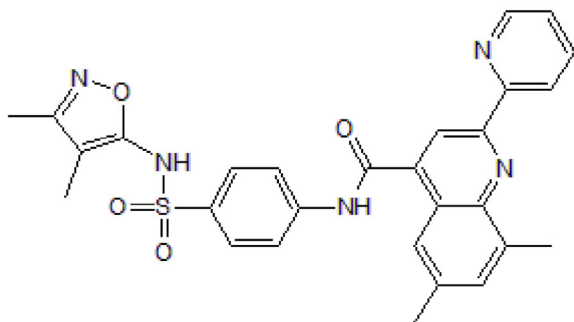
Batch Molecular Formula: C₂₈H₂₅N₅O₄S.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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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