Print Date: Mar 15th 2022

Certificate of Analysis

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Product Name: **CID 2745687** **Catalog No.: 4293** **Batch No.: 2**

CAS Number: 264233-05-8

IUPAC Name: 1-(2,4-Difluorophenyl)-5-[[2-[[(1,1-dimethylehyl)amino]thioxomethyl]hydrazinylidene]methyl]-1*H*-pyrazole-4-carboxylic acid methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{19}F_2N_5O_2S$

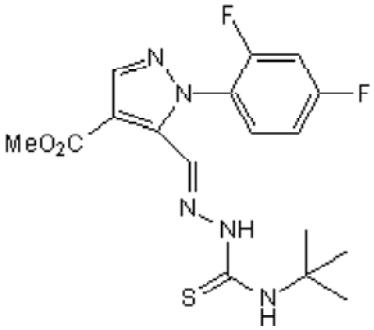
Batch Molecular Weight: 395.43

Physical Appearance: Cream solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.64	4.84	17.71
Found	51.62	4.84	17.74

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Description:

CID 2745687 is a competitive, reversible antagonist of the orphan receptor GPR35 (K_i = 12.8 nM). Blocks the GPR35-mediated increase in ERK1/2 phosphorylation and β-arrestin recruitment induced by pamoic acid.

Physical and Chemical Properties:

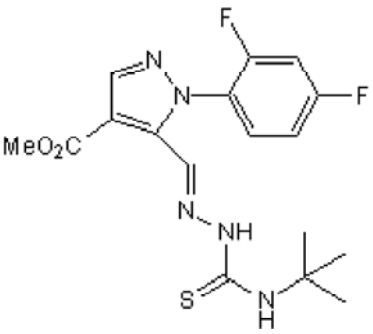
Batch Molecular Formula: $C_{17}H_{19}F_2N_5O_2S$

Batch Molecular Weight: 395.43

Physical Appearance: Cream solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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°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:

Jenkins *et al* (2012) Antagonists of GPR35 display high species ortholog selectivity and varying modes of action. J.Pharmacol.Exp.Ther. ***343*** 683. PMID: 22967846.

Zhao *et al* (2010) Targeting of the orphan receptor GPR35 by pamoic acid: a potent activator of extracellular signal-regulated kinase and β-arrestin2 with antinociceptive activity. Mol.Pharmacol. ***78*** 560. PMID: 20826425.