

Product Name: KML 29

Catalog No.: 4872

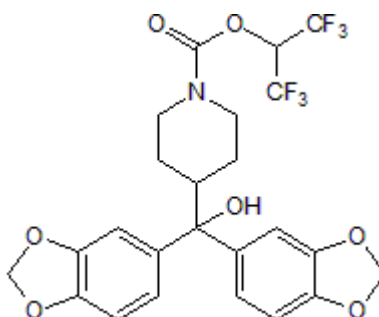
Batch No.: 1

CAS Number: 1380424-42-9

IUPAC Name: 4-[Bis(1,3-benzodioxol-5-yl)hydroxymethyl]-1-piperidinecarboxylic acid 2,2,2-trifluoro-1-(trifluoromethyl)ethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₁F₆NO₇
Batch Molecular Weight: 549.42
Physical Appearance: White powder
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Ethyl acetate:Petroleum ether [4:1])
HPLC: Shows >99.1% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.47	3.85	2.55
Found	52.45	3.77	2.72

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

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Description:

Highly selective and potent monoacylglycerol lipase (MAGL) inhibitor. Exhibits potent inhibition of human, mouse and rat MAGL (IC₅₀ values are 5.9, 15 and 43 nM, respectively). Exhibits no detectable inhibition of FAAH (IC₅₀ > 50000 nM). Potently and selectively blocks hydrolysis of 2-arachidonoylglycerol (2-AG) in mice (IC₅₀ = 2.5 nM and >50 μM for 2-AG and AEA respectively).

Physical and Chemical Properties:

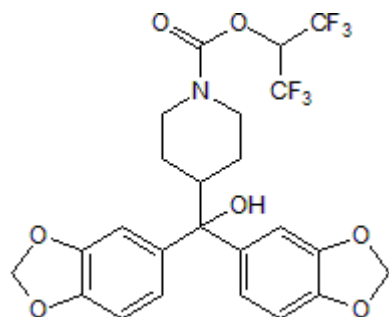
Batch Molecular Formula: C₂₄H₂₁F₆NO₇

Batch Molecular Weight: 549.42

Physical Appearance: White powder

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:

Ueda *et al* (2012) Discrimination between two endocannabinoids. *Chem.Biol.* **19** (5) 545. PMID: 22633404.

Chang *et al* (2012) Highly selective inhibitors of monoacylglycerol lipase bearing a reactive group that is bioisosteric with endocannabinoid substrates. *Chem.Biol.* **19** (5) 579. PMID: 22542104.

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