TOCRIS
a bio-techne brand

Print Date: Apr 30th 2016

Certificate of Analysis

www.tocris.com

Product Name: **KML 29** **Catalog No.: 4872** **Batch No.: 3**

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: $C_{24}H_{21}F_6NO_7$

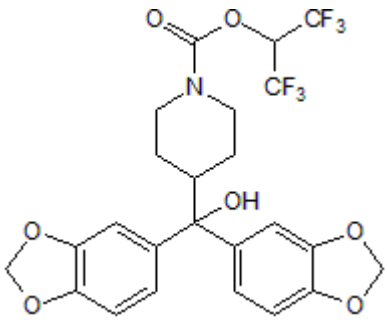
Batch Molecular Weight: 549.42

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.27 (Ethyl acetate:Petroleum ether [4:1])

HPLC: Shows >98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.47	3.85	2.55
Found	52.66	3.98	2.73

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Name: **KML 29** **Catalog No.: 4872** **Batch No.: 3**

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

Description:

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

Physical and Chemical Properties:

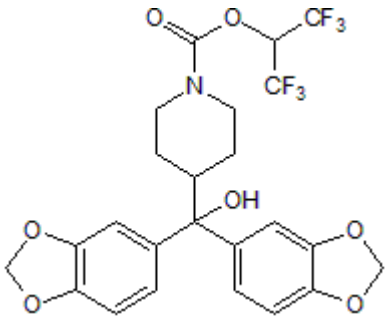
Batch Molecular Formula: $C_{24}H_{21}F_6NO_7$

Batch Molecular Weight: 549.42

Physical Appearance: Off 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:

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

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