

**Product Name:** JJKK 048

**Catalog No.:** 5206

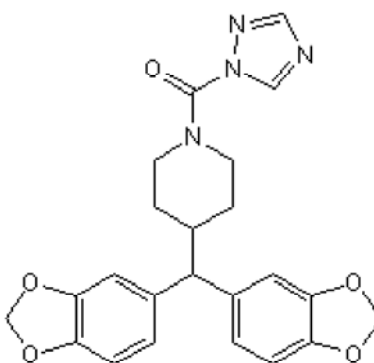
**Batch No.:** 1

CAS Number: 1515855-97-6

IUPAC Name: 4-[Bis(1,3-benzodioxol-5-yl)methyl]-1-piperidiny]-1*H*-1,2,4-triazol-1-yl-methanone

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>23</sub>H<sub>22</sub>N<sub>4</sub>O<sub>5</sub>  
**Batch Molecular Weight:** 434.44  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.37 (Chloroform:Methanol:Ammonia soln. [90:9:1])  
**HPLC:** Shows 97.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	63.59	5.1	12.9
Found	63.54	5.18	12.56

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

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**Description:**

Potent and selective monoacylglycerol lipase (MAGL) inhibitor ( $IC_{50} = 0.4$  nM). Exhibits >13,000 and ~630-fold selectivity for MAGL over FAAH and ABHD6, respectively. Increases brain levels of 2-arachidonoylglycerol (2-AG) levels in mice in vivo. Promotes analgesia in pain models.

**Physical and Chemical Properties:**

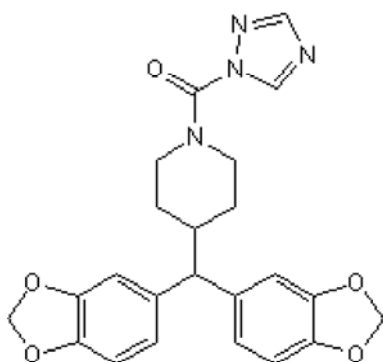
Batch Molecular Formula:  $C_{23}H_{22}N_4O_5$

Batch Molecular Weight: 434.44

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:**

**Aaltonen et al (2016)** *In vivo* characterization of the ultrapotent monoacylglycerol lipase inhibitor {4-[bis-(benzo[d][1,3]dioxol-5-yl)methyl]-piperidin-1-yl}(1H-1,2,4-triazol-1-yl)methanone (JJKK-048). *J.Pharmacol.Exp.Ther.* **359** 62. PMID: 27451409.

**Laitinen et al (2014)** Mutation of Cys242 of human monoacylglycerol lipase disrupts balanced hydrolysis of 1- and 2-monoacylglycerols and selectively impairs inhibitor potency. *Mol.Pharmacol.* **85** 510. PMID: 24368842.

**Aaltonen et al (2013)** Piperazine and piperidine triazole ureas as ultrapotent and highly selective inhibitors of monoacylglycerol lipase. *Chem.Biol.* **20** 379. PMID: 23521796.

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