

# **Certificate of Analysis**

Print Date: Jan 14<sup>th</sup> 2016

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Product Name: JW 642 Catalog No.: 4906 Batch No.: 1

CAS Number: 1416133-89-5

IUPAC Name: 4-[(3-Phenoxyphenyl)methyl]-1-piperazinecarboxylic acid 2,2,2-trifluoro-1-(trifluoromethyl)ethyl ester

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{21}H_{20}F_6N_2O_3$ 

**Batch Molecular Weight:** 462.39 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

# 2. ANALYTICAL DATA

**HPLC:** Shows >99.7% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.55 4.36 6.06 Found 54.74 4.35 6.16



# **Product Information**

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**IUPAC Name:** 4-[(3-Phenoxyphenyl)methyl]-1-piperazinecarboxylic acid 2,2,2-trifluoro-1-(trifluoromethyl)ethyl ester

## **Description:**

Potent and selective monoacylglycerol lipase (MAGL) inhibitor (IC<sub>50</sub> = 3.7 nM). Displays >1000-fold selectivity for MAGL over fatty acid amide hydrolase (IC<sub>50</sub> = 20.6  $\mu$ M). Analog of JZL 195 (Cat. No. 4715).

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>21</sub>H<sub>20</sub>F<sub>6</sub>N<sub>2</sub>O<sub>3</sub> Batch Molecular Weight: 462.39 Physical Appearance: White solid

# Minimum Purity: >98%

#### **Batch Molecular Structure:**

Storage: Store at -20°C

### Solubility & Usage Info:

DMSO to 100 mM ethanol 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.

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