

# **Certificate of Analysis**

Print Date: Nov 2<sup>nd</sup> 2016

www.tocris.com

Product Name: BMS 986187 Catalog No.: 5983 Batch No.: 1

CAS Number: 684238-37-7

IUPAC Name: 3,4,5,6,7,9-Hexahydro-3,3,6,6-tetramethyl-9-[4-[(2-methylphenyl)methoxy]phenyl]-1*H*-xanthene-1,8(2*H*)-dione

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{31}H_{34}O_4$ . <sup>1</sup>/<sub>4</sub> $H_2O$ 

**Batch Molecular Weight:** 475.11 **Physical Appearance:** White solid

Solubility: DMSO to 20 mM Storage: Store at +4°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 99.3% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 78.37 7.32 Found 78.53 7.19



# **Product Information**

Print Date: Nov 2<sup>nd</sup> 2016

www.tocris.com

Product Name: BMS 986187 Catalog No.: 5983 Batch No.: 1

CAS Number: 684238-37-7

IUPAC Name: 3,4,5,6,7,9-Hexahydro-3,3,6,6-tetramethyl-9-[4-[(2-methylphenyl)methoxy]phenyl]-1*H*-xanthene-1,8(2*H*)-dione

# **Description:**

Potent  $\delta$ -opioid receptor positive allosteric modulator (EC<sub>50</sub> = 30 nM). Exhibits 100-fold selectivity for  $\delta$  over  $\mu$ -opioid receptor. Enhances affinity of [Leu<sup>5</sup>]-Enkephalin (Cat.No. 1889), SNC 80 (Cat.No. 0764) and TAN 67 (Cat.No. 0921) for the  $\delta$ -opioid receptor.

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

Batch Molecular Formula:  $C_{31}H_{34}O_4$ .  $\frac{1}{4}H_2O_4$ 

Batch Molecular Weight: 475.11 Physical Appearance: White solid

**Minimum Purity: >98%** 

# **Batch Molecular Structure:**

Storage: Store at +4°C

# Solubility & Usage Info:

DMSO to 20 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:

**Shang** et al (2016) Proposed mode of binding and action of positive allosteric modulators at opioid receptors. ACS Chem.Biol. 11 1220. PMID: 26841170.

**Burford** *et al* (2015) Discovery, synthesis, and molecular pharmacology of selective positive allosteric modulators of the δ-opioid receptor. J.Med.Chem. *58* 4220. PMID: 25901762.