



# **Certificate of Analysis**

www.tocris.com

**Product Name:** SB 216641 hydrochloride Catalog No.: 1242 Batch No.: 6

CAS Number: 193611-67-5

**IUPAC Name:** N-[3-[3-(Dimethylamino)ethoxy]-4-methoxyphenyl]-2'-methyl-4'-(5-methyl-1,2,4-oxadiazol-3-yl)-[1,1'-biphenyl]-4-

carboxamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{28}H_{30}N_4O_4.HCI.\frac{1}{2}H_2O$ 

532.04 **Batch Molecular Weight: Physical Appearance:** White solid Solubility: water to 50 mM Store at RT Storage:

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

TLC:  $R_f = 0.16$  (Dichloromethane:Methanol [95:5])

HPLC: Shows 98.8% purity <sup>1</sup>H NMR: Consistent with structure **Mass Spectrum:** Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 63.21 6.06 10.53 Found 63.35 5.92 10.42

Tel: +44 (0)1235 529449 www.tocris.com/distributors Tel:+1 612 379 2956



# **Product Information**

Print Date: Nov 14th 2017

Batch No.: 6

www.tocris.com

Product Name: SB 216641 hydrochloride

CAS Number: 193611-67-5

IUPAC Name: N-[3-[3-(Dimethylamino)ethoxy]-4-methoxyphenyl]-2'-methyl-4'-(5-methyl-1,2,4-oxadiazol-3-yl)-[1,1'-biphenyl]-4-

carboxamide hydrochloride

#### **Description:**

A selective h5-HT $_{\rm 1B}$  antagonist with approximately 25-fold selectivity over h5-HT $_{\rm 1D}$  and little or no affinity for a range of other receptor types.

# **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>28</sub>H<sub>30</sub>N<sub>4</sub>O<sub>4</sub>.HCl.½H<sub>2</sub>O

Batch Molecular Weight: 532.04 Physical Appearance: White solid

Minimum Purity: >98%

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

Storage: Store at RT

#### Solubility & Usage Info:

water to 50 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).

Catalog No.: 1242

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.

## **Licensing Information:**

Sold with the permission of GlaxoSmithKline

#### References:

**Hagan** et al (1997) Stimulation of 5-HT<sub>1B</sub> receptors causes hypothermia in the guinea pig. Eur.J.Pharmacol. **331** 169. PMID: 9274976.

**Price** *et al* (1997) SB-216641 and BRL-15572 - compounds to pharmacologically discriminate h5-HT<sub>1B</sub> and h5-HT<sub>1D</sub> receptors. Naunyn Schmiedebergs Arch.Pharmacol. *356* 312. PMID: 930567.

**Schlicker** *et al* (1997) Effects of selective h5-HT<sub>1B</sub> (SB-216641) and 5-HT<sub>1D</sub> (BRL-15572) receptor ligands on guinea pig and human 5-HT auto- and heteroreceptors. Naunyn Schmiedebergs Arch.Pharmacol. *356* 321. PMID: 9303568.