

## **Certificate of Analysis**

Print Date: Feb 11th 2022

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Product Name: SB 277011A dihydrochloride Catalog No.: 4207 Batch No.: 4

CAS Number: 1226917-67-4

IUPAC Name: N-[trans-4-[2-(6-Cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-quinolinecarboxamide dihydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>30</sub>N<sub>4</sub>O.2HCl.1<sup>1</sup>/<sub>4</sub>H<sub>2</sub>O

Batch Molecular Weight: 534.01

Physical Appearance: Off White solid

Solubility: DMSO to 50 mM

Storage: Store at +4°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 98.9% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen Chlorine

Theoretical 62.98 6.51 10.49 13.28 Found 63.2 6.11 10.36 12.86



### **Product Information**

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### **Description:**

SB 277011A dihydrochloride is a selective dopamine  $D_3$  receptor antagonist (pK<sub>i</sub> values are 8.0, 6.0, 5.0 and <5.2 for  $D_3$ ,  $D_2$ , 5-HT<sub>1D</sub> and 5-HT<sub>1B</sub> respectively). Brain penetrant.

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

Batch Molecular Formula: C<sub>28</sub>H<sub>30</sub>N<sub>4</sub>O.2HCl.1½H<sub>2</sub>O

Batch Molecular Weight: 534.01 Physical Appearance: Off White solid

# **Minimum Purity:** ≥98%

### **Batch Molecular Structure:**

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Catalog No.: 4207

### Solubility & Usage Info:

DMSO 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).

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 for research purposes under agreement from GlaxoSmithKline.

### References:

**Reavill** et al (2000) Pharmacological actions of a novel, high-affinity, and selective human DA  $D_3$  receptor antagonist, SB-277011-A. J.Pharmacol.Exp.Ther. **294** 1154. PMID: 10945872.

**Stemp** *et al* (2000) Design and synthesis of trans-N-[4-[2-(6-cyano-1,2,3,4-tetrahydroisoquinolin-2-yl)ethyl]cyclohexyl]-4-quinolinecarboxamide (SB-277011): a potent and selective DA D3 receptor antagonist with high oral bioavailability and CNS pe J.Med.Chem. *43* 1878. PMID: 10794704.

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