



# **Certificate of Analysis**

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Product Name: bPiDDB Catalog No.: 3221 Batch No.: 1

CAS Number: 525596-66-1

IUPAC Name: 1,1'-(1,12-Dodecanediyl)bis[3-methylpyridinium] dibromide

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{24}H_{38}Br_2N_2$ .  $^{1/2}H_2O$ 

Batch Molecular Weight: 523.39

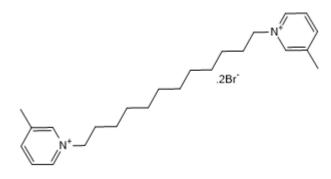
Physical Appearance: Light brown lyophilised solid

**Solubility:** water to 100 mM

DMSO to 100 mM

Storage: Desiccate at RT

**Batch Molecular Structure:** 



#### 2. ANALYTICAL DATA

**HPLC:** Shows 100% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.08 7.51 5.35 Found 54.96 7.52 5.35



# **Product Information**

Print Date: Apr 19<sup>th</sup> 2016 **WWW.tocris.com** 

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CAS Number: 525596-66-1

IUPAC Name: 1,1'-(1,12-Dodecanediyl)bis[3-methylpyridinium] dibromide

## **Description:**

Orthosteric neuronal nicotinic acetylcholine receptor (nAChR) antagonist (IC $_{50}$  values are 0.17, 0.25, 0.4, 4.8, 6.5, 8.2, 20 and 34  $\mu\text{M}$  at  $\alpha3\beta4$ ,  $\alpha1\beta1\epsilon\bar{b}$ ,  $\alpha3\beta4\beta3$ ,  $\alpha6\beta4\beta3$ ,  $\alpha7$ ,  $\alpha4\beta2$ ,  $\alpha3\beta2\beta3$  and  $\alpha6/3\beta2\beta3$  receptors respectively). Attenuates nicotine-evoked dopamine release from the ventral tegmental area in vivo (IC $_{50}$  = 0.2 nM) and reduces nicotine self-administration in rats. Brain penetrant.

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

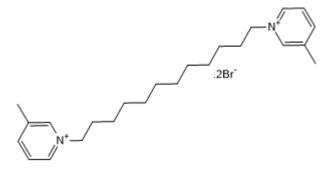
Batch Molecular Formula: C<sub>24</sub>H<sub>38</sub>Br<sub>2</sub>N<sub>2</sub>.1/2H<sub>2</sub>O

Batch Molecular Weight: 523.39

Physical Appearance: Light brown lyophilised solid

Minimum Purity: >98%

## **Batch Molecular Structure:**



**Storage:** Desiccate at RT. This product is packaged under an inert atmosphere.

#### Solubility & Usage Info:

water to 100 mM DMSO to 100 mM

CAUTION: This product is extremely hygroscopic.

# 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:

**Dwoskin** *et al* (2008) *N,N'*alkane-diyl-*bis*-3-picoliniums as nicotinic receptor antagonists: Inhibition of nicotine-evoked dopamine release and hyperactivity. J.Pharmacol.Exp.Ther. *326* 563. PMID: 18460644.

**Rahman** *et al* (2008) Region-specific effects of the *N,N'*-dodecane-1,12-diyl-bis-3-picolinium dibromide on nicotine-induced increase in extracellular dopamine *in vivo*. Br.J.Pharmacol. *153* 792. PMID: 18059317.

**Ayers** *et al* (2002) Bis-azaaromatic quaternary ammonium analogues: ligands for  $\alpha 4\beta 2^*$  and  $\beta 7^*$  subtypes of neuronal nicotinic receptors Bioorg.Med.Chem.Letts. **12** 3067.