

Certificate of Analysis

Print Date: May 19th 2022

www.tocris.com

Product Name: TCB-2 Catalog No.: 2592 Batch No.: 6

CAS Number: 912342-28-0

IUPAC Name: (4-Bromo-3,6-dimethoxybenzocyclobuten-1-yl)methylamine hydrobromide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₁H₁₄BrNO₂.HBr.

Batch Molecular Weight: 353.05

Physical Appearance: White solid

Solubility: water to 25 mM

DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 37.42 4.28 3.97 Found 37.62 4.28 3.96



Product Information

Print Date: May 19th 2022

www.tocris.com

Product Name: TCB-2 Catalog No.: 2592 Batch No.: 6

CAS Number: 912342-28-0

IUPAC Name: (4-Bromo-3,6-dimethoxybenzocyclobuten-1-yl)methylamine hydrobromide

Description:

TCB-2 is a high affinity 5-HT $_{2A}$ receptor agonist (K $_{i}$ values are 0.73 and 0.75 nM for rat and human receptors respectively). Potently stimulates IP $_{3}$ accumulation in NIH3T3 cells stably expressing rat 5-HT $_{2A}$ receptors (EC $_{50}$ = 36 nM). Induces head twitches and hypothermia in mice following i.p. administration.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₁H₁₄BrNO₂.HBr.

Batch Molecular Weight: 353.05 Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

water to 25 mM DMSO 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:

Niebert et al (2011) Expression and function of serotonin 2A and 2B receptors in the mammalian respiratory network. PLoS One 6 e21395. PMID: 21789169.

Fox *et al* (2010) The serotonin 5-HT_{2A} receptor agonist TCB-2: a behavioral and neurophysiological analysis. Psychopharmacology *212* 13. PMID: 19823806.

McLean *et al* (2006) 1-Aminomethylbenzocycloalkanes: conformationally restricted hallucinogenic phenethylamine analogues as functionally selective 5-HT_{2A} receptor agonists. J.Med.Chem. *49* 5794. PMID: 16970404.