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Certificate of Analysis

www.tocris.com

Catalog No.: 2532

Print Date: Feb 26th 2024

Batch No.: 1

Product Name: TFB-TBOA

CAS Number: 480439-73-4 IUPAC Name: (3S)-3-[[3-[[4-

: (3S)-3-[[3-[[4-(Trifluoromethyl)benzoyl]amino]phenyl]methoxy]-L-aspartic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight:

Physical Appearance:

Solubility:

Storage:

Batch Molecular Structure:

C₁₉H₁₇F₃N₂O₆.H₂O 444.37 White solid DMSO to 50 mM Store at -20°C



2. ANALYTICAL DATA

HPLC: Chiral HPLC: ¹H NMR: Mass Spectrum: Microanalysis: Shows >99.1% purity Shows >99.9% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 51.36 4.31 6.3 Found 51.6 4.39 6.24

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

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CAS Number: 480439-73-4

IUPAC Name:

(3S)-3-[[3-[[4-(Trifluoromethyl)benzoyl]amino]phenyl]methoxy]-L-aspartic acid

Description:

TFB-TBOA is a potent and selective glial glutamate transporter EAAT1 and EAAT2 inhibitor (IC_{50} values are 17, 22 and 300 nM for EAAT2, EAAT1 and EAAT3, respectively). Exhibits selectivity for EAAT1 and EAAT2 over EAAT4 and EAAT5, and a wide range of neuronal receptors and transporters. In HEK293 cells expressing human EAAT1, 2, and 3, TFB-TBOA exhibited selectivity for hEAAT1 and hEAAT2 over hEAAT3 (respective IC_{50} values are 3.6, 10, and 120 nM), while in tsA201 cells expressing rat EAAT4, [³H]-d-Asp uptake was inhibited with an IC_{50} of 40 nM. Attenuates glutamate-stimulated intracellular Na⁺ elevation in astrocytes in vitro ($IC_{50} = 43$ nM). ... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{19}H_{17}F_3N_2O_6.H_2O$ Batch Molecular Weight: 444.37 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM

When purchased as a 1mg unit, this product is supplied in lyophilized form. It may appear as a solid, gel or film and be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Fu *et al* (2018) Chemoenzymatic synthesis and pharmacological characterization of functionalized aspartate analogues as novel excitatory amino acid transporter inhibitors. J.Med.Chem. **61** 7741. PMID: 30011368.

Magi *et al* (2012) Physical and functional interaction of NCX1 and EAAC1 transporters leading to glutamate-enhanced ATP production in brain mitochondria. PLoS One **7** e34015. PMID: 22479505.

Bozzo and Chatton (2010) Inhibitory effects of (2S, 3S)-3-[3-[4-(trifluoromethyl)benzoylamino]benzyloxy]aspartate (TFB-TBOA) on the astrocytic sodium responses to glutamate. Brain Res. **1316** (27). PMID: 20026319.

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