

# **Certificate of Analysis**

Print Date: Jan 15th 2016

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Product Name: WAY 213613 Catalog No.: 2652 Batch No.: 1

CAS Number: 868359-05-1

IUPAC Name: N-[4-(2-Bromo-4,5-difluorophenoxy)phenyl]-L-asparagine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{16}H_{13}BrF_2N_2O_4$ 

Batch Molecular Weight: 415.19

Physical Appearance: Off-white solid

Solubility: 1eq. NaOH to 100 mM

DMSO to 100 mM

Storage: Desiccate at RT

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.78$  (Pyridine:Acetic acid:Water:Butanol [3:8:11:15])

HPLC: Shows 99.8% purity
Chiral HPLC: Shows 99.9% purity

14 NMP: Consistent with structure.

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

**Optical Rotation:**  $[\alpha]_D = -6$  (Concentration = 1, Solvent = DMSO)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 46.29 3.16 6.74 Found 45.97 3.27 6.54



# **Product Information**

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**IUPAC Name:** N-[4-(2-Bromo-4,5-difluorophenoxy)phenyl]-L-asparagine

# **Description:**

Potent, non-substrate inhibitor of EAAT2 (GLT-1) that displays > 44-fold selectivity over EAAT1 and EAAT3 (IC50 values are 85, 3787 and 5004 nM for EAAT2, EAAT3 and EAAT1 respectively). Exhibits no activity towards ionotropic and metabotropic glutamate receptors.

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

Batch Molecular Formula: C<sub>16</sub>H<sub>13</sub>BrF<sub>2</sub>N<sub>2</sub>O<sub>4</sub> Batch Molecular Weight: 415.19 Physical Appearance: Off-white solid

Minimum Purity: >99%

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

$$\begin{array}{c|c} F & & H & CO_2H \\ \hline \\ & O & NH_2 \\ \end{array}$$

Storage: Desiccate at RT

## Solubility & Usage Info:

1eq. NaOH to 100 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:

Dunlop et al (2005) Characterization of novel aryl-ether, biaryl, and fluorene aspartic acid and diaminopropionic acid analogs as potent inhibitors of the high-affinity glutamate transporter EAAT2. Mol. Pharmacol. 68 974. PMID: 16014807.

Beart and Shea (2007) Transporters for L-glutamate: an update on their molecular pharmacology and pathological involvement. Br.J.Pharmacol. 150 5. PMID: 17088867.