



# **Certificate of Analysis**

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Product Name: IP7e Catalog No.: 5699 Batch No.: 1

CAS Number: 500164-74-9

IUPAC Name: 6-[4-[(2-Methoxyethoxy)methyl]phenyl]-5-methyl-3-phenyl-isoxazolo[4,5-c]pyridin-4(5H)-one

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{22}N_2O_4$ Batch Molecular Weight:390.43Physical Appearance:White solid

**Solubility:** DMSO to 100 mM

ethanol to 20 mM with gentle warming

Storage: Store at +4°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.37$  (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 98.7% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.75 5.68 7.17 Found 71.07 5.67 7.14



# **Product Information**

Print Date: May 27th 2016

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## **Description:**

Potent Nurr1 activator (EC $_{50}$  = 3.9 nM). Delays onset and reduces severity of symptoms in mice with experimental autoimmune encephalomyelitis (EAE). Also suppresses NF-кВ signaling. Brain penetrant and orally bioavailable.

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

Batch Molecular Formula: C23H22N2O4 Batch Molecular Weight: 390.43 Physical Appearance: White solid

Minimum Purity: >98%

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

Storage: Store at +4°C

### Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 mM with gentle warming

#### 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:

Montarolo et al (2014) Effects of isoxazolo-pyridinone 7e, a potent activator of the Nurr1 signaling pathway, on experimental autoimmune encephalomyelitis in mice. PLoS One 9 e108791. PMID: 25265488.

Hintermann et al (2007) Identification of a series of highly potent activators of the Nurr1 signaling pathway. Bioorg.Med.Chem.Lett. 17 193. PMID: 17035009.

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