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Print Date: Jan 26th 2016

Certificate of Analysis

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Product Name: **PNU 120596** **Catalog No.: 2498** **Batch No.: 3**

CAS Number: 501925-31-1

IUPAC Name: *N*-(5-Chloro-2,4-dimethoxyphenyl)-*N*'-(5-methyl-3-isoxazolyl)-urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{14}ClN_3O_4$

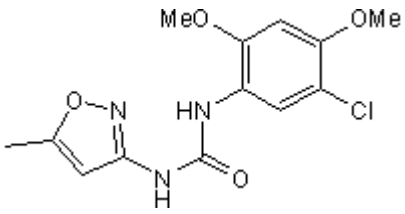
Batch Molecular Weight: 311.72

Physical Appearance: White fluffy solid

Solubility: DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.66 (Chloroform:Methanol [9:1])

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.09	4.53	13.48
Found	49.93	4.47	13.47

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Description:

Positive allosteric modulator of α7 neuronal nicotinic acetylcholine receptors (EC_{50} = 216 nM), with no detectable effect on α4β2, α3β4 and α9α10 receptors. Active in vivo following systemic administration. Neuroprotective in an in vivo model of transient focal cerebral ischemia.

Physical and Chemical Properties:

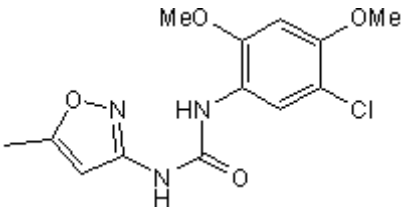
Batch Molecular Formula: $C_{13}H_{14}ClN_3O_4$

Batch Molecular Weight: 311.72

Physical Appearance: White fluffy solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

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:

Hurst *et al* (2005) A novel positive allosteric modulator of the α7 neuronal nicotinic acetylcholine receptor: *in vitro* and *in vivo* characterization. J.Neurosci. ***25*** 4396. PMID: 15858066.

Timmermann *et al* (2007) An allosteric modulator of the α7 nicotinic acetylcholine receptor possessing cognition-enhancing properties in vivo. J.Pharmacol.Exp.Ther. ***323*** 294. PMID: 17625074.

Kalappa *et al* (2013) A positive allosteric modulator of α7 nAChRs augments neuroprotective effects of endogenous nicotinic agonists in cerebral ischemia. Br.J.Pharmacol. [Epub ahead of print]. PMID: 23713819.

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