



# **Certificate of Analysis**

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Product Name: (R)-(-)-Niguldipine hydrochloride Catalog No.: 1124 Batch No.: 1

CAS Number: 113145-70-3

IUPAC Name: (R)-1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic acid, 3-(4,4-diphenyl-1-piperidinyl)propyl

methyl ester hydrochloride

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{36}H_{39}N_3O_6.HCl.$ <sup>3</sup>/<sub>4</sub>H<sub>2</sub>O

Batch Molecular Weight: 659.6914

Physical Appearance: Yellow solid

Solubility: water to 10 mM

Storage: Desiccate at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.5$  (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

Melting Point:

Between 150 - 153°C

TH NMR:

Consistent with structure

**Optical Rotation:**  $[\alpha]_D = -14$  (Concentration = 1, Solvent = MeOH)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 65.54 6.34 6.36 0 0 0 0 Found 65.48 6.22 6.35 0 0 0



# **Product Information**

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Print Date: Jan 15th 2016

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methyl ester hydrochloride

#### **Description:**

L-type  $Ca^{2+}$  channel blocker and  $\alpha_{1A}$ -adrenoceptor antagonist; less active enantiomer. (S)-(+)-Niguldipine hydrochloride (Cat. No. 1123) also available.

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

Batch Molecular Formula:  $C_{36}H_{39}N_3O_6.HCI.34H_2O$ 

Batch Molecular Weight: 659.6914 Physical Appearance: Yellow solid

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

Storage: Desiccate at -20°C

### Solubility & Usage Info:

water to 10 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:

**Boer** *et al* (1989) (+)-Niguldipine binds with very high affinity to Ca<sup>2+</sup> channels and to a subtype of alpha<sub>1</sub>-adrenoceptor. Eur.J.Pharmacol. *172* 131. PMID: 2548881.

**Graziadei** *et al* (1989) Stereoselective binding of niguldipine enantiomers to alpha<sub>1A</sub>-adrenoceptors labeled with [3H]5-methyl-urapidil. Eur.J.Pharmacol. *172* 329. PMID: 2555206.

Hollt et al (1992) Stereoisomers of calcium antagonists which differ markedly in their potencies as calcium blockers are equally effective in modulating drug transport by P-glycoprotein. Biochem.Pharmacol. 43 2601. PMID: 1352973.

Wetzel et al (1995) Discovery of alpha<sub>1a</sub>-adrenergic receptor antagonists based on the L-type Ca<sup>2+</sup> channel antagonist niguldipine. J Med Chem. **38** 1579 PMID: 7752182