

**Product Name:** (S)-(+)-Niguldipine hydrochloride

**Catalog No.:** 1123

**Batch No.:** 1

**CAS Number:** 113145-69-0

**IUPAC Name:** (S)-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:**  $C_{36}H_{39}N_3O_6 \cdot HCl \cdot \frac{1}{2}H_2O$

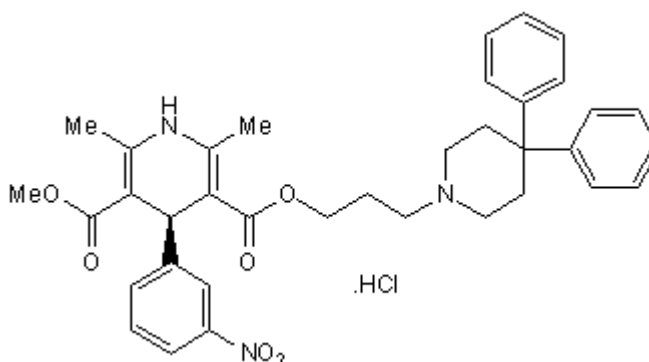
**Batch Molecular Weight:** 655.1876

**Physical Appearance:** Yellow solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Desiccate at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.8$  (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

**Melting Point:** Between 159 - 161°C

**<sup>1</sup>H NMR:** Consistent with structure

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

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen		
Theoretical	65.99	6.31	6.41	0	0
Found	65.61	6.21	6.29	0	0

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**Description:**

L-type Ca<sup>2+</sup> channel blocker and α<sub>1A</sub>-adrenoceptor antagonist; more active enantiomer. (R)-(-)-Niguldipine hydrochloride (Cat. No. 1124) also available.

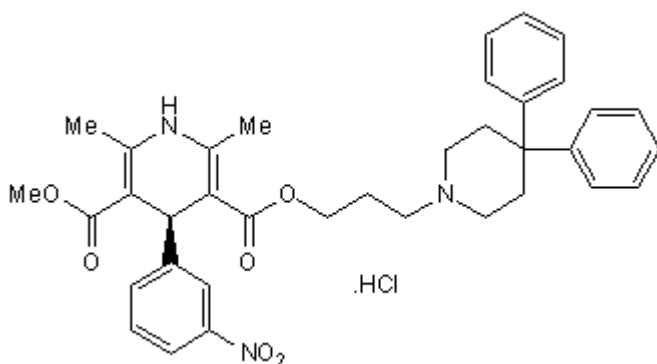
**Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>36</sub>H<sub>39</sub>N<sub>3</sub>O<sub>6</sub>.HCl.½H<sub>2</sub>O

Batch Molecular Weight: 655.1876

Physical Appearance: Yellow solid

**Batch Molecular Structure:**



**Storage:** Desiccate at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol 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:**

**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 [<sup>3</sup>H]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.

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