

Product Name: SNAP 5089

Catalog No.: 2398

Batch No.: 1

CAS Number: 157066-77-8

IUPAC Name: 5-[[[3-(4,4-Diphenyl-1-piperidiny)propyl]amino]carbonyl]-1,4-dihydro-2,6-dimethyl-4-(4-nitrophenyl)-3-pyridinecarboxylic acid methyl ester hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₆H₄₀N₄O₅·HCl·1½H₂O

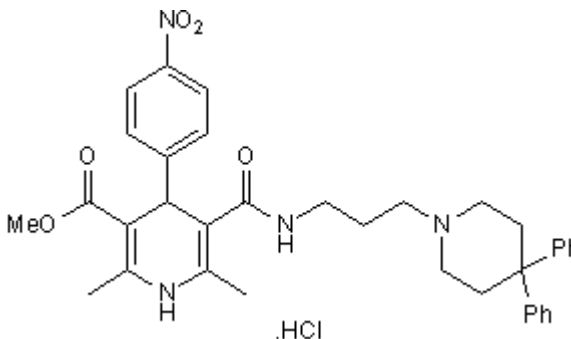
Batch Molecular Weight: 672.21

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >98% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	64.32	6.6	8.33	5.27
Found	64.38	6.38	8.34	4.87

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Description:

Subtype-selective α_{1A} -adrenoceptor antagonist that displays > 600-fold selectivity over other adrenoceptors (K_i values are 0.35, 220, 370, 540, 800 and 1200 nM for α_{1A} , α_{1B} , α_{2C} , α_{1D} , α_{2B} and α_{2A} subtypes respectively and 540 nM for L-type Ca^{2+} channels). Inhibits noradrenalin-induced contractions in rabbit vascular and lower urinary tissues.

Physical and Chemical Properties:

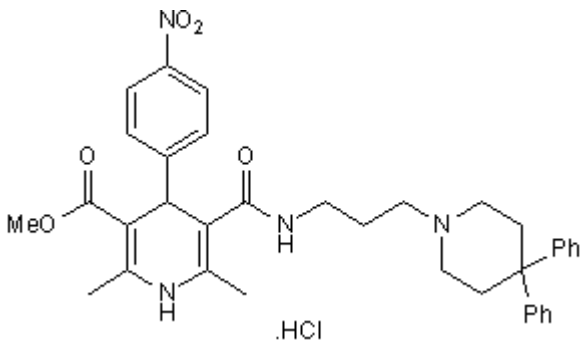
Batch Molecular Formula: $C_{36}H_{40}N_4O_5 \cdot HCl \cdot 1 \frac{1}{2} H_2O$

Batch Molecular Weight: 672.21

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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:

Wetzel et al (1995) Discovery of α_{1A} -adrenergic receptor antagonists based on the L-type Ca^{2+} channel antagonist niguldipine. *J.Med.Chem.* **38** 1579. PMID: 7752182.

Leonardi et al (1997) Pharmacological characterization of the uroselective α_1 -antagonist Rec 15-2739 (SB 216469): role of the α_1 -1L adrenoceptor in tissue selectivity, Part I. *J.Pharmacol.Exp.Ther.* **281** 1272. PMID: 9190863.

Kava et al (1998) α_{1L} -adrenoceptor mediation of smooth muscle contraction in rabbit bladder neck: a model for lower urinary tract tissues of man. *Br.J.Pharmacol.* **123** 1359. PMID: 9579731.

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