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Certificate of Analysis

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Product Name: SKF 89976A hydrochloride

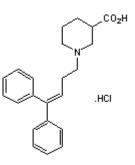
Catalog No.: 1081 Batch No.: 1

CAS Number: IUPAC Name: 85375-15-1 1-(4,4-Diphenyl-3-butenyl)-3-piperidinecarboxylic acid hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₂₂H₂₅NO₂.HCl 371.91 White solid water to 100 mM with gentle warming DMSO to 100 mM Desiccate at +4°C

Storage: Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: Melting Point: HPLC: ¹H NMR: Microanalysis: R_f = 0.4 (Dichloromethane:Methanol:Ammonia soln. [8:2:0:2]) Between 184 - 186°C Shows 100% purity Consistent with structure

Carbon Hydrogen Nitrogen						
Theoretical	71.05	7.05	3.77	000		
Found	71.09	7.16	3.9	000		

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Print Date: Jan 15th 2016

Batch No.: 1

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CAS Number: 85375-15-1

IUPAC Name: 1-(4,4-Diphenyl-3-butenyl)-3-piperidinecarboxylic acid hydrochloride

Description:

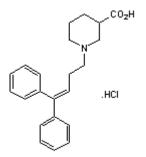
A potent GABA uptake inhibitor, selective for GAT-1 (IC₅₀ values are 0.13, 550, 944 and 7210 μ M for hGAT-1, rGAT-2, hGAT-3 and hBGT-1 respectively). Inhibits transport current competitively (K_i = 7 μ M) and transmitter-gated current non-competitively (K_i = 0.03 nM). Able to pass the blood-brain barrier after systemic administration and is active in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₂H₂₅NO₂.HCl Batch Molecular Weight: 371.91 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 100 mM with gentle warming 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).

Catalog No.: 1081

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:

Ali et al (1985) Orally active and potent inhibitors of y-aminobutyric acid. J.Med.Chem. 28 653. PMID: 2985785.

Murali Dha (1996) On the bioactive conformation of the GABA uptake inhibitor SK&F 89976-A. Bioorg.Med.Chem.Lett. 6 1535.

Krause and Schwarz (2005) Identification and selective inhibition of the channel mode of the neuronal GABA transporter 1. Mol.Pharmacol. 68 1728. PMID: 16150932.

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