

Certificate of Analysis

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Product Name: PRE-084 hydrochloride

Catalog No.: 0589

Batch No.: 2

CAS Number: 138847-85-5

IUPAC Name: 2-(4-Morpholinethyl) 1-phenylcyclohexanecarboxylate hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₇NO₃.HCl

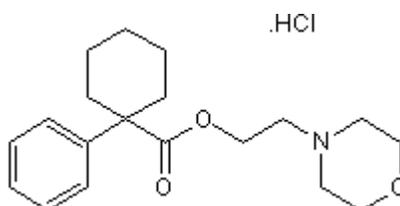
Batch Molecular Weight: 353.89

Physical Appearance: Cream solid

Solubility: water to 25 mM
DMSO to 75 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

UV Spectrum: Consistent with structure

	Carbon Hydrogen Nitrogen		
	Carbon	Hydrogen	Nitrogen
Theoretical	64.49	7.97	3.96
Found	64.56	8.09	3.91

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

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IUPAC Name: 2-(4-Morpholinethyl) 1-phenylcyclohexanecarboxylate hydrochloride

Description:

High affinity, selective σ_1 agonist (K_i values are 2.2 and 13091 nM for σ_1 and σ_2 receptors respectively). Selective over PCP receptors ($IC_{50} > 100000$ nM) and several other receptor systems. Produces anti-amnesic and antitussive effects in vivo. Also exhibits protective effects in PC6.3 cells expressing mutant huntingtin by activating NF- κ B signaling.

Physical and Chemical Properties:

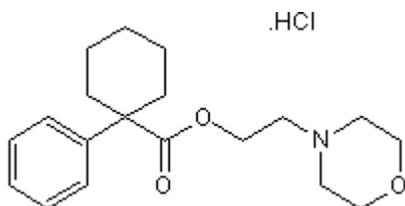
Batch Molecular Formula: $C_{19}H_{27}NO_3 \cdot HCl$

Batch Molecular Weight: 353.89

Physical Appearance: Cream solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

water to 25 mM

DMSO to 75 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:

Hyrskyluoto et al (2013) Sigma-1 receptor agonist PRE084 is protective against mutant huntingtin-induced cell degeneration: involvement of calpastatin and the NF- κ B pathway. *Cell Death Dis.* **4** e646. PMID: 23703391.

Brown et al (2004) Antitussive activity of sigma-1 receptor agonists in the guinea-pig. *Br.J.Pharmacol.* **141** 233. PMID: 14691051.

Maurice et al (1999) The attenuation of learning impairments induced after exposure to CO or trimethyltin in mice by sigma (σ) receptor ligands involves both σ_1 and σ_2 sites. *Br.J.Pharmacol.* **127** 335. PMID: 10385231.

Su et al (1991) Sigma compounds derived from phencyclidine. Identification of PRE-084, a new selective sigma ligand. *J.Pharmacol.Exp.Ther.* **259** 543. PMID: 1658302.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956