

Certificate of Analysis

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Product Name: XE 991 dihydrochloride

Catalog No.: 2000

Batch No.: 2

CAS Number: 122955-13-9

IUPAC Name: 10,10-*bis*(4-Pyridinylmethyl)-9(10*H*)-anthracenone dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₀N₂O.2HCl.¼H₂O

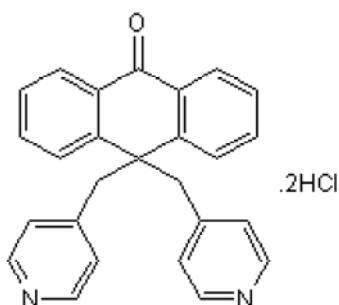
Batch Molecular Weight: 453.87

Physical Appearance: Off-white solid

Solubility: water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.24 (Chloroform:Methanol [95:5])

HPLC: Shows 99% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.8	5	6.17
Found	68.65	4.85	6.19

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

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IUPAC Name: 10,10-bis(4-Pyridinylmethyl)-9(10H)-anthracenone dihydrochloride

Description:

Potent and selective blocker of K_v7 (KCNQ) voltage-gated potassium channels. Blocks K_v7.2+7.3 (KCNQ2+3) / M-currents (IC₅₀ = 0.6 - 0.98 μM) and K_v7.1 (KCNQ1) homomeric channels (IC₅₀ = 0.75 μM) but is less potent against K_v7.1/minK channels (IC₅₀ = 11.1 μM). Augments hippocampal ACh release and is a cognitive enhancer following oral administration in vivo.

Physical and Chemical Properties:

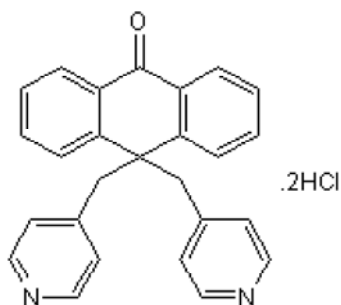
Batch Molecular Formula: C₂₆H₂₀N₂O.2HCl.¼H₂O

Batch Molecular Weight: 453.87

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Passmore et al (2003) KCNQ/M currents in sensory neurons: significance for pain therapy. *J.Neurosci.* **23** 7227. PMID: 12904483.

Wang et al (2000) Molecular basis for differential sensitivity of KCNQ and I_{Ks} channels to the cognitive enhancer XE991. *Mol.Pharmacol.* **57** 1218. PMID: 10825393.

Wang et al (1998) KCNQ2 and KCNQ3 potassium channel subunits: molecular correlates of the M-channel. *Science* **282** 1890. PMID: 9836639.

Zaczek et al (1998) Two new potent neurotransmitter release enhancers, 10,10-bis(4-pyridinylmethyl)-9(10H)-anthracenone and 10,10-bis(2-fluoro-4-pyridinylmethyl)-9(10H)-anthracenone: comparison to linopirdine. *J.Pharmacol.Exp.Ther.* **285** 724. PMID: 9580619.

Storage: Desiccate at RT

Solubility & Usage Info:

water 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.

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