

Certificate of Analysis

Print Date: Oct 13th 2022

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Product Name: Trequinsin hydrochloride Catalog No.: 2337 Batch No.: 1

CAS Number: 78416-81-6

IUPAC Name: 2,3,6,7-Tetrahydro-9,10-dimethoxy-3-methyl-2-[(2,4,6-trimethylphenyl)imino]-4*H*-pyrimido[6,1-a]isoquinolin-4-one

hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₇N₃O₃.HCl

Batch Molecular Weight: 441.95

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.2$ (Ether:Petroleum ether [2:1])

HPLC: Shows 96.6% purity

¹H NMR: Consistent with structure

¹³C NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 65.22 6.39 9.5 Found 64.95 6.46 9.32



Product Information

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Description:

Trequinsin hydrochloride is a highly potent inhibitor of cGMP-inhibited phosphodiesterase (PDE3; IC $_{50}$ = 250 pM). Potently inhibits arachidonic acid-induced aggregation of human platelets (IC $_{50}$ = 50 pM). Orally active antihypertensive agent; reduces systemic blood pressure in both normotensive and hypertensive animal models. Also activates CatSper channels, increases intracellular Ca $^{2+}$ and cGMP levels, and decreases potassium channel activity in sperm.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₄H₂₇N₃O₃.HCl

Batch Molecular Weight: 441.95

Physical Appearance: Pale yellow solid

Minimum Purity: ≥97%

Batch Molecular Structure:

Storage: Desiccate at RT

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).

Catalog No.: 2337

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:

McBrinn *et al* (2019) Novel pharmacological actions of Trequinsin Hydrochloride improve human sperm cell motility and function. Br.J.Pharmacol.. PMID: 31368510.

Agarwal *et al* (1987) Role of plasma adenosine in the antiplatelet action of HL 725, a potent inhibitor of cAMP phosphodiesterase: species differences. Thromb.Res. *47* 191. PMID: 2821650.

Lal *et al* (1984) Trequinsin, a potent new antihypertensive vasodilator in the series of 2-(arylimino)-3-alkyl-9,10-dimethoxy-3,4,6,7-tetrahydro-2*H*-pyrimido[6,1-a]isoquinolin-4-ones. J.Med.Chem. **27** 1470. PMID: 6492077.

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