

Product Name: Zosuquidar trihydrochloride

Catalog No.: 5456

Batch No.: 1

CAS Number: 167465-36-3

IUPAC Name: (*αR*)-4-[(1*α*,6*α*,10*β*)-1,1-Difluoro-1,1*a*,6,10*b*-tetrahydrodibenzo[*a,e*]cyclopropa[*c*]cyclohepten-6-yl]-*α*-[(5-quinolinyl)oxy)methyl]-1-piperazineethanol trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₂H₃₁F₂N₃O₂·3HCl·4½H₂O

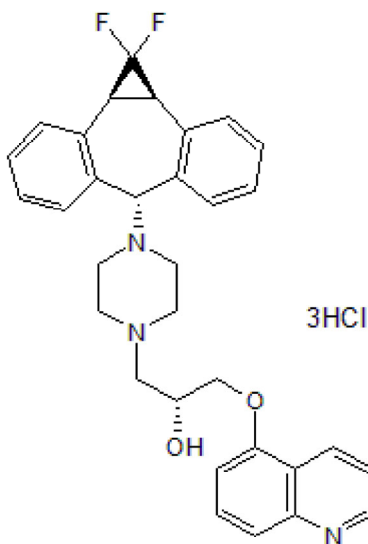
Batch Molecular Weight: 718.06

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 53.53 | 6.04 | 5.85 |
| Found | 53.26 | 5.88 | 5.83 |

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Description:

Zosuquidar trihydrochloride is a high affinity P-glycoprotein (P-gp) inhibitor (K_d = 79 nM). Restores doxorubicin (Cat. No. 2252) sensitivity in P-gp-expressing multidrug (MDR) resistant cancer cell lines. Also potentiates antitumor efficacy of taxol (Cat. No. 1097) in a MDR human non-small cell lung carcinoma xenograft mouse model.

Physical and Chemical Properties:

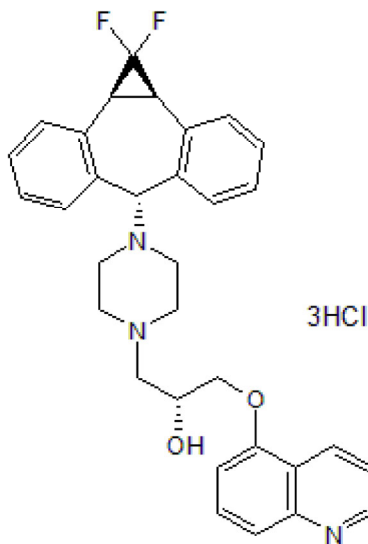
Batch Molecular Formula: C₃₂H₃₁F₂N₃O₂·3HCl·4½H₂O

Batch Molecular Weight: 718.06

Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



References:

Dantzig et al (1999) Selectivity of the multidrug resistance modulator, LY335979, for P-glycoprotein and effect on cytochrome P-450 activities. *J.Pharmacol.Exp.Ther.* **290** 854. PMID: 10411602.

Dantzig et al (1996) Reversal of P-glycoprotein-mediated multidrug resistance by a potent cyclopropyldibenzosuberane modulator, LY335979. *Cancer Res.* **56** 4171. PMID: 8797588.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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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