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Print Date: Jan 15th 2016

Certificate of Analysis

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Product Name: **XR 9051 HCl** **Catalog No.: 2944** **Batch No.: 1**

CAS Number: 180422-22-4

IUPAC Name: *N*-[4-[2-(3,4-Dihydro-6,7-dimethoxy-2(1*H*)-isoquinolinyl)ethyl]phenyl]-3-[(*Z*)-[(5*Z*)-4-methyl-3,6-dioxo-5-(phenylmethylene)piperazinylidene]methyl]benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{39}H_{38}N_4O_5.HCl.1¾H_2O$

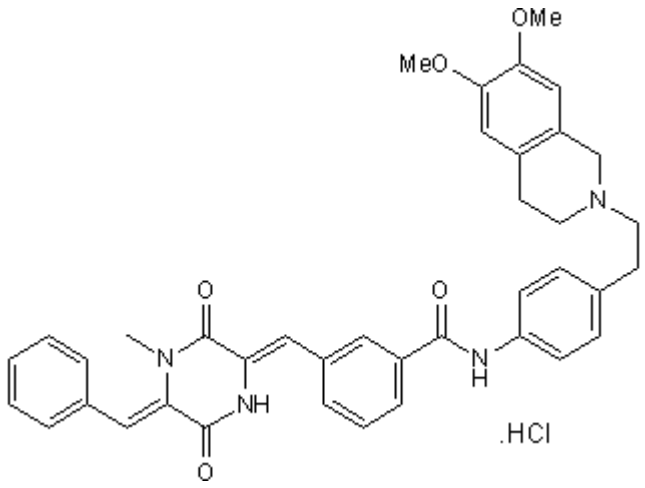
Batch Molecular Weight: 710.72

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.3% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.91	6.03	7.88
Found	65.78	5.5	7.89

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Description:

Potent modulator of P-glycoprotein-mediated multidrug resistance (MDR) that inhibits the binding of cytotoxics to P-glycoprotein (EC_{50} = 134 nM). Reverses resistance to a variety of cytotoxic drugs (including doxorubicin, etoposide and vincristine) in several murine and human P-gp-overexpressing cell lines. Orally active.

Physical and Chemical Properties:

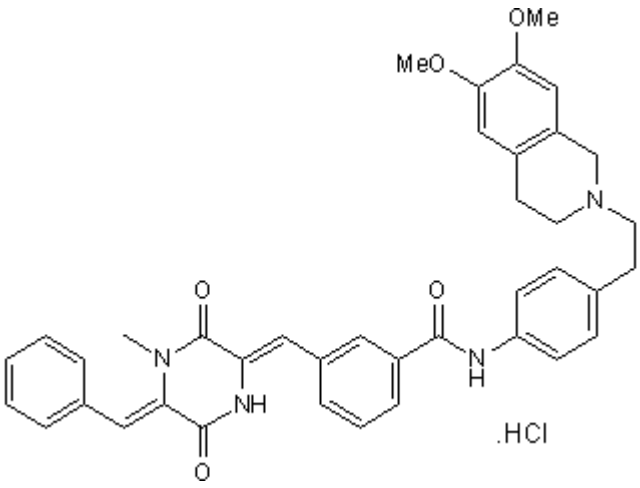
Batch Molecular Formula: $C_{39}H_{38}N_4O_5.HCl.1¾H_2O$

Batch Molecular Weight: 710.72

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

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).

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:

Dale *et al* (1998) Reversal of P-glycoprotein-mediated multidrug resistance by XR9051, a novel diketopiperazine derivative. Br.J.Cancer ***78*** 885. PMID: 9764579.

Mistry *et al* (1999) In vivo efficacy of XR9051, a potent modulator of P-glycoprotein mediated multidrug resistance. Br.J.Cancer ***79*** 1672. PMID: 10206276.

Martin *et al* (2000) Communication between multidrug binding sites on P-glycoprotein. Mol.Pharmacol. ***58*** 624. PMID: 10953057.