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Print Date: Jan 15th 2016

Certificate of Analysis

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Product Name: **CP 100356 hydrochloride** **Catalog No.: 4193** **Batch No.: 1**

CAS Number: 142715-48-8

IUPAC Name: 4-(3,4-Dihydro-6,7-dimethoxy-2(1*H*)-isoquinolinyl)-*N*-2[2-(3,4-dimethoxyphenyl)ethyl]-6,7-dimethoxy-2-quinazolinamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{31}H_{36}N_4O_6.HCl$

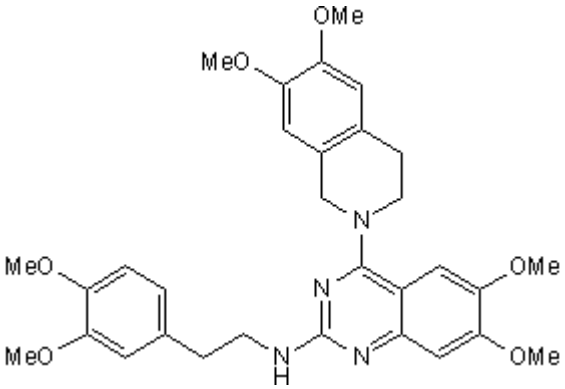
Batch Molecular Weight: 597.1

Physical Appearance: Off-white solid

Solubility: DMSO to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.36	6.25	9.38
Found	62.17	6.42	9.36

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Product Information

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Description:

High affinity P-glycoprotein (P-gp) inhibitor (K_i values are 58 and 94 nM for mouse Pgp1a and Pgp1b isoforms). Inhibits calcein-AM uptake in MDR1-transfected MDCKII cells (IC_{50} = 0.5 µM) and prazosin transport in BCRP-transfected MDCKII cells (IC_{50} = 1.5 µM). Displays weak or no inhibitory activity against MRP1, OATP1B1 and several major human P450 enzymes (IC_{50} > 50 µM).

Physical and Chemical Properties:

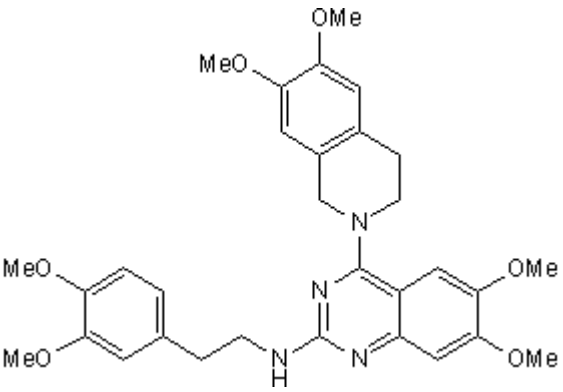
Batch Molecular Formula: $C_{31}H_{36}N_4O_6.HCl$

Batch Molecular Weight: 597.1

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 20 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:

Taylor *et al* (1999) The equilibrium and kinetic drug binding properties of the mouse P-gp1a and P-gp1b P-glycoproteins are similar. Br.J.Cancer ***81*** 783. PMID: 10555746.

Wandel *et al* (1999) P-glycoprotein and cytochrome P-450 3A inhibition: dissociation of inhibitory potencies. Cancer Res. ***59*** 3944. PMID: 10463589.

Kalgutkar *et al* (2009) *N*-(3,4-dimethoxyphenethyl)-4-(6,7-dimethoxy-3,4-dihydroisoquinolin-2[1*H*]-yl)-6,7-dimethoxyquinazolin-2-amine (CP-100,356) as a "chemical knock-out equivalent" to assess the impact of efflux transporters on oral drug absorption in the rat. J.Pharm.Sci. ***98*** 4914. PMID: 19373887.

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