Certificate of Analysis

Product Name: **LY 333531 hydrochloride** **Catalog No.: 4738** **Batch No.: 3**

CAS Number: 169939-93-9

IUPAC Name: (9*S*)-9-[(Dimethylamino)methyl]-6,7,10,11-tetrahydro-9*H*,18*H*-5,21:12,17-dimethenodibenzo[*e*,*k*]pyrrolo[3,4-*h*][1,4,13]oxadiazacyclohexadecine-18,20(19*H*)-dione hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{28}N_4O_3.HCl$

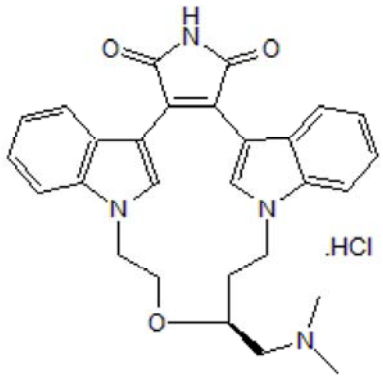
Batch Molecular Weight: 505.01

Physical Appearance: Red solid

Solubility: DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Name: **LY 333531 hydrochloride** **Catalog No.: 4738** **Batch No.: 3**

CAS Number: 169939-93-9

IUPAC Name: (9*S*)-9-[(Dimethylamino)methyl]-6,7,10,11-tetrahydro-9*H*,18*H*-5,21:12,17-dimethenodibenzo[*e*,*k*]pyrrolo[3,4-*h*][1,4,13]oxadiazacyclohexadecine-18,20(19*H*)-dione hydrochloride

Description:

Isozyme-selective inhibitor of protein kinase C (PKC); competitively and reversibly inhibits PKCβI and PKCβII (IC_{50} values are 4.7 and 5.9 nM respectively). Selective for PKCβ over other PKC isozymes (IC_{50} values are 0.052, 0.25, 0.30, 0.36, 0.60 and >100 μM for PKCη, -δ, -γ, -α, -ε and -ζ respectively). Exhibits selectivity for PKC over other ATP-dependent kinases, including protein kinase A, casein kinase and src).

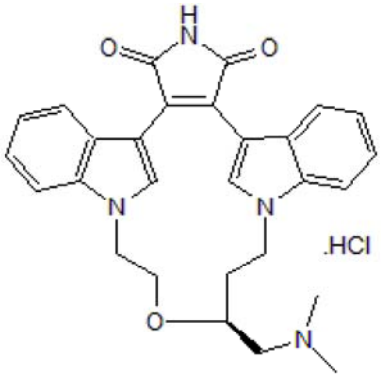
Physical and Chemical Properties:

Batch Molecular Formula: $C_{28}H_{28}N_4O_3$.HCl

Batch Molecular Weight: 505.01

Physical Appearance: Red solid

Batch Molecular Structure:



Storage: Store at -20°C. This product is packaged under an inert atmosphere.

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 20 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Lewin *et al* (2018) Synthesis and Characterization of the Selective, Reversible PKCß Inhibitor (9S)-9-[(Dimethylamino)methyl]-6,7,10,11-tetrahydro-9H,18H-5,21:12,17-dimethenodibenzo[e,k]pyrrolo[3,4-h][1,4,13]oxadiazacyclohexadecine-18,20(19H)-dione, Ruboxistaurin (LY333531) A.C.S.Chem.Neurosci..

Faul *et al* (2003) Acyclic *N*-(azacycloalkyl)bisindolylmaleimides: isozyme selective inhibitors of PKCβ. Bioorg.Med.Chem.Lett. ***13*** 1857. PMID: 12749884.

Samokhin *et al* (1999) Effects of protein kinase C inhibitors on thromboxane production by thrombin-stimulated platelets. Eur.J.Pharmacol. ***386*** 297. PMID: 10618482.

Jirousek *et al* (1996) (*S*)-13-[(dimethylamino)methyl]-10,11,14,15-tetrahydro-4,9:16,21-dimetheno-1*H*,13*H*-dibenzo[*e*,*k*]]pyrrolo[3,4-*h*][1,4,13]oxadiazacyclohexadecene-1,3(2*H*)-dione (LY333531) and related analogues: isozyme selective inhibitors of protein kinase Cβ. J.Med.Chem. ***39*** 2664. PMID: 8709095.