TOCRIS
a bio-techne brand

Print Date: Jan 8th 2016

Certificate of Analysis

www.tocris.com

Product Name: **KN-62** **Catalog No.: 1277** **Batch No.: 8**

CAS Number: 127191-97-3

IUPAC Name: 4-[(2*S*)-2-[(5-isoquinolinylsulfonyl)methylamino]-3-oxo-3-(4-phenyl-1-piperazinyl)propyl] phenyl isoquinolinesulfonic acid ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{38}H_{35}N_5O_6S_2.½H_2O$

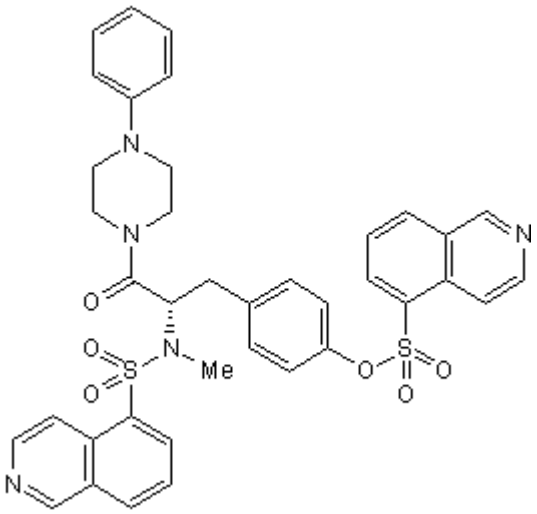
Batch Molecular Weight: 730.85

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.32 (Chloroform:Methanol [95:5])

HPLC: Shows 99.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.45	4.96	9.58
Found	62.36	4.87	9.41

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Description:

Selective, cell-permeable inhibitor of CaM kinase II (IC_{50} = 0.9 µM). Binds directly to the calmodulin binding site of the enzyme. Potent non-competitive antagonist at the $P2X_7$ receptor (IC_{50} = 15 nM).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{38}H_{35}N_5O_6S_2.½H_2O$

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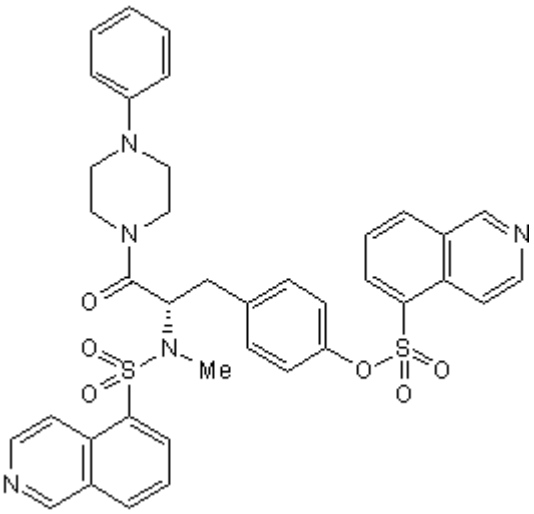
Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 100 mM

This product may be supplied in a sealed glass ampoule, please refer to the Tocris catalogue for opening instructions. 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:

Tokumitsu *et al* (1990) KN-62, 1-[N-O-bis(5-isoquinolinesulfonyl)-N-methyl-L-tyrosyl]-4-phenylpiperazine, a specific inhibitor of Ca^{2+}/calmodulin-dependent protein kinase II. J.Biol.Chem. ***265*** 4315. PMID: 2155222.

Hidaka and Yokokura (1996) Molecular and cellular pharmacology of a calcium/calmodulin-dependent protein kinase II (CaM kinase II) inhibitor, KN-62, and proposal of CaM kinase phosphorylation cascades. Adv.Pharmacol. ***36*** 193. PMID: 8783561.

Chessell *et al* (1998) Effects of antagonists at the human recombinant $P2X_7$ receptor. Br.J.Pharmacol. ***124*** 1314. PMID: 9720806.