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Certificate of Analysis

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Product Name: KN-62

Catalog No.: 1277 Batch No.: 9

CAS Number: 127191-97-3 IUPAC Name: 4-[(2S)-2-[(5-

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage:

Batch Molecular Structure:

C₃₈H₃₅N₅O₆S₂.¼H₂O 726.34 Pale yellow solid DMSO to 100 mM Store at -20°C



2. ANALYTICAL DATA HPLC: Chiral HPLC: ¹H NMR:

Mass Spectrum: Microanalysis: Shows 98.3% purity Shows 100% purity Consistent with structure Consistent with structure

	Carbonn	yurogenn	litiogei
Theoretical	62.84	4.93	9.64
Found	62	4.69	9.65

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name:

127191-97-3 4-[(2:S)-2-[(5-i)

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

Description:

CAS Number:

KN-62 is a selective, cell-permeable inhibitor of CaM kinase II (IC₅₀ = 0.9 μ M). Binds directly to the calmodulin binding site of the enzyme. Potent non-competitive antagonist at the P2X₇ receptor (IC₅₀ = 15 nM).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{38}H_{35}N_5O_6S_2$.¹/₄H₂O Batch Molecular Weight: 726.34 Physical Appearance: Pale yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Chessell *et al* (1998) Effects of antagonists at the human recombinant P2X₇ receptor. Br.J.Pharmacol. **124** 1314. PMID: 9720806.

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.

Tokumitsu *et al* (1990) KN-62, 1-[N-O-bis(5-isoquinolinesulfonyl)-N-methyl-L-tyrosyl]-4-phenylpiperazine, a specific inhibitor of Ca²⁺/calmodulin-dependent protein kinase II. J.Biol.Chem. **265** 4315. PMID: 2155222.

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Storage: Store 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.