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

CAS Number: 127191-97-3
IUPAC Name: 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: \( \text{C}_{38}\text{H}_{35}\text{N}_{5}\text{O}_{6}\text{S}_{2}\cdot\frac{1}{2}\text{H}_{2}\text{O} \)
Batch Molecular Weight: 730.85
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM
Storage: Desiccate at -20°C

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:
<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>62.45</td>
<td>4.96</td>
<td>9.58</td>
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<tr>
<td>Found</td>
<td>62.36</td>
<td>4.87</td>
<td>9.41</td>
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</table>
**Product Name:** KN-62  
**CAS Number:** 127191-97-3  
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**Description:**
Selective, cell-permeable inhibitor of CaM kinase II (IC₅₀ = 0.9 μM). 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:** C₃₈H₃₆N₂O₈S₂.H₂O
- **Batch Molecular Weight:** 730.85
- **Physical Appearance:** Pale yellow solid
- **Minimum Purity:** >98%

**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.

**Storage:** Desiccate at -20°C

**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 Ca²⁺/calmodulin-dependent protein kinase II. J.Biol.Chem. 265 4315. PMID: 2155222.