Print Date: Jan 15th 2016

# Certificate of Analysis

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**Product Name:** **KC 12291 hydrochloride** **Catalog No.: 3251** **Batch No.: 1**

CAS Number: 181936-98-1

IUPAC Name: 3,4-Dimethoxy-*N*-methyl-*N*-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]benzeneethanamine hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{22}H_{27}N_3O_3S.HCl.¼H_2O$

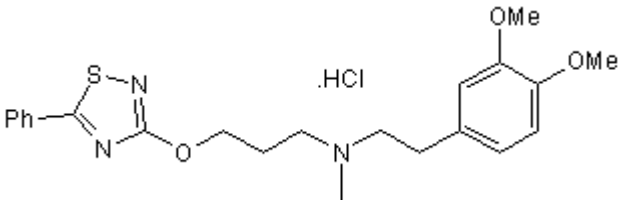
**Batch Molecular Weight:** 454.49

**Physical Appearance:** Off-white solid

**Solubility:** water to 25 mM
DMSO to 50 mM
ethanol to 10 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**HPLC:** Shows 97.7% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 58.14 | 6.32 | 9.25 |
| Found | 58.08 | 6.18 | 9.16 |



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**Description:**

Orally active atypical voltage-gated sodium channel blocker. Inhibits sustained sodium currents ($I_{NaL}$) and prevents diastolic contracture in isolated atria in vitro ($IC_{50}$ values are 9.6 and 0.55 - 0.79 µM respectively). Displays anti-ischemic, bradycardic and cardioprotective activity in vivo.

**Physical and Chemical Properties:**

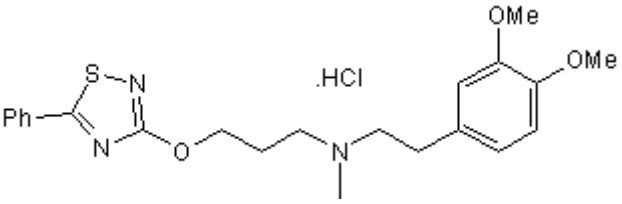
Batch Molecular Formula: $C_{22}H_{27}N_3O_3S.HCl.¼H_2O$

Batch Molecular Weight: 454.49

Physical Appearance: Off-white solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**




**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

water to 25 mM
DMSO to 50 mM
ethanol to 10 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:**

**Decking** *et al* (1998) Cardioprotective actions of KC 12291. Naunyn-Schmied.Arch.Pharmacol. ***358*** 547.

**Tamareille** *et al* (2002) Anti-ischemic compound KC 12291 prevents diastolic contracture in isolated atria by blockade of voltage-gated sodium channels. J.Cardiovasc.Pharmacol. ***40*** 346. PMID: 12198320.

**John** *et al* (2004) KC 12291: an atypical sodium channel blocker with myocardial antiischemic properties. Cardiovasc.Drug Rev. ***22*** 17. PMID: 14978516.

**Letienne** *et al* (2006) Pharmacological characterisation of sodium channels in sinoatrial node pacemaking in the rat heart. Eur.J.Pharmacol. ***530*** 243. PMID: 16368090.



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