

**Product Name:** A 804598

**Catalog No.:** 4473

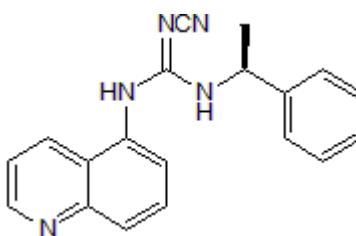
**Batch No.:** 2

CAS Number: 1125758-85-1

IUPAC Name: *N*-Cyano-*N'*-[(1*S*)-1-phenylethyl]-*N*-5-quinolinyl-guanidine

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>19</sub>H<sub>17</sub>N<sub>5</sub>  
**Batch Molecular Weight:** 315.37  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.6 (Dichloromethane:Methanol [95:5])  
**HPLC:** Shows >99.9% purity  
**Chiral HPLC:** Shows >99.5% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	72.36	5.43	22.21
Found	72.06	5.55	21.96

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

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**Description:**

Potent, competitive P2X<sub>7</sub> receptor antagonist (IC<sub>50</sub> values are 8.9, 9.9 and 10.9 nM for mouse, rat and human P2X<sub>7</sub> receptors respectively). Selective for P2X<sub>7</sub> receptors (IC<sub>50</sub> > 5-10 μM for a wide array of cell surface receptors and ion channels). Binds with high affinity (K<sub>i app</sub> = 2.4 nM for rat P2X<sub>7</sub> receptors).

**Physical and Chemical Properties:**

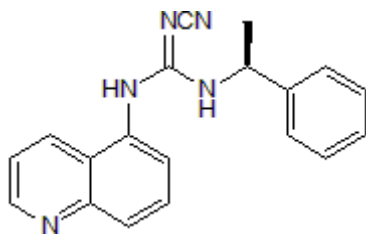
Batch Molecular Formula: C<sub>19</sub>H<sub>17</sub>N<sub>5</sub>

Batch Molecular Weight: 315.37

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Donnelly-Roberts et al** (2009) [3H]A-804598 ([3H]2-cyano-1-[(1*S*)-1-phenylethyl]-3-quinolin-5-ylguanidine) is a novel, potent, and selective antagonist radioligand for P2X<sub>7</sub> receptors. *Neuropharmacology* **56** 223. PMID: 18602931.

**Able et al** (2011) Receptor localization, native tissue binding and ex vivo occupancy for centrally penetrant P2X<sub>7</sub> antagonists in the rat. *Br.J.Pharmacol.* **162** 405. PMID: 20840537.

**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 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.

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**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