

Product Name: A 804598

Catalog No.: 4473

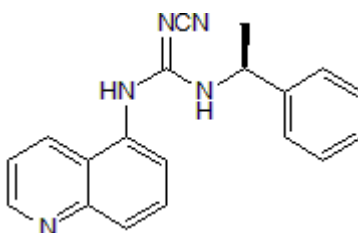
Batch No.: 2

CAS Number: 1125758-85-1

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₇N₅
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_f = 0.6 (Dichloromethane:Methanol [95:5])
HPLC: Shows >99.9% purity
Chiral HPLC: Shows >99.5% purity
¹H 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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CAS Number: 1125758-85-1

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

Description:

Potent, competitive P2X₇ receptor antagonist (IC₅₀ values are 8.9, 9.9 and 10.9 nM for mouse, rat and human P2X₇ receptors respectively). Selective for P2X₇ receptors (IC₅₀ > 5-10 μM for a wide array of cell surface receptors and ion channels). Binds with high affinity (K_{i app} = 2.4 nM for rat P2X₇ receptors).

Physical and Chemical Properties:

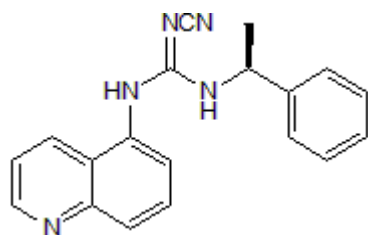
Batch Molecular Formula: C₁₉H₁₇N₅

Batch Molecular Weight: 315.37

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



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.

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 P2X₇ receptors. *Neuropharmacology* **56** 223. PMID: 18602931.

Able et al (2011) Receptor localization, native tissue binding and ex vivo occupancy for centrally penetrant P2X₇ antagonists in the rat. *Br.J.Pharmacol.* **162** 405. PMID: 20840537.

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