

Product Name: JNJ 47965567

Catalog No.: 5299

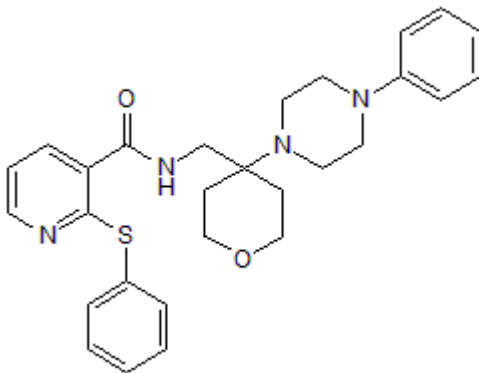
Batch No.: 2

CAS Number: 1428327-31-4

IUPAC Name: 2-(Phenylthio)-N-[[tetrahydro-4-(4-phenyl-1-piperazinyl)-2H-pyran-4-yl]methyl-3-pyridinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₃₂N₄O₂S
Batch Molecular Weight: 488.64
Physical Appearance: White powder
Solubility: 1eq. HCl to 50 mM
DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [95:5])
HPLC: Shows >99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 68.82 | 6.6 | 11.47 |
| Found | 68.88 | 6.67 | 11.44 |

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

Product Name: JNJ 47965567

Catalog No.: 5299

Batch No.: 2

CAS Number: 1428327-31-4

IUPAC Name: 2-(Phenylthio)-N-[[tetrahydro-4-(4-phenyl-1-piperazinyl)-2H-pyran-4-yl]methyl-3-pyridinecarboxamide

Description:

Potent and selective P2X₇ antagonist (pIC₅₀ values are 8.3, 7.5 and 7.2 for human, mouse and rat receptors respectively). Selective over a panel of 50 other receptors, ion channels and transporters. Reduces BzATP-induced IL-1 β release from monocytes in vitro and from rat brain in vivo. Attenuates amphetamine-induced hyperactivity in rats. Brain penetrant.

Physical and Chemical Properties:

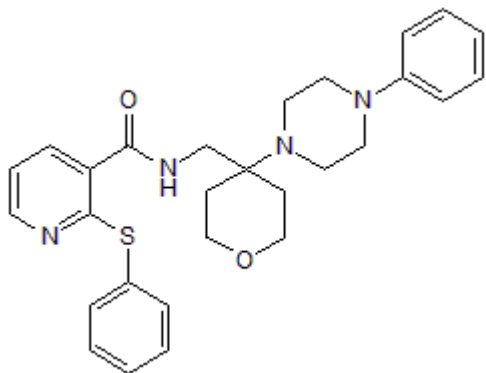
Batch Molecular Formula: C₂₈H₃₂N₄O₂S

Batch Molecular Weight: 488.64

Physical Appearance: White powder

Minimum Purity: >98%

Batch Molecular Structure:



References:

Bhattacharya et al (2013) Pharmacological characterization of a novel centrally permeable P2X₇ receptor antagonist: JNJ-47965567. Br.J.Pharmacol. **170** 624. PMID: 23889535.

Letavic et al (2013) Synthesis and pharmacological characterization of two novel, brain penetrating P2X₇ antagonists. ACS Med.Chem.Lett. **12** 419. PMID: 24900687.

Storage: Store at +4°C

Solubility & Usage Info:

1eq. HCl to 50 mM
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.

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

Tocris Bioscience is an R&D Systems company

USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373

www.RnDSystems.com