

Product Name: JNJ 47965567

Catalog No.: 5299

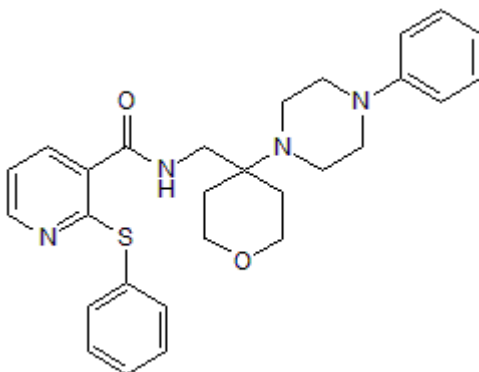
Batch No.: 5

CAS Number: 1428327-31-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

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



2. ANALYTICAL DATA

TLC: R_f = 0.43 (Dichloromethane:Methanol [95:5])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.82	6.6	11.47
Found	68.49	6.89	11.42

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

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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-1β release from monocytes in vitro and from rat brain in vivo. Attenuates amphetamine-induced hyperactivity in rats. Brain penetrant.

Physical and Chemical Properties:

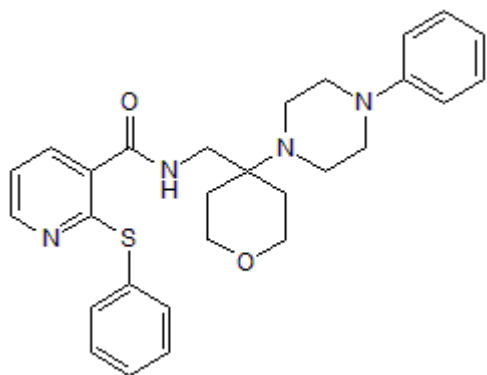
Batch Molecular Formula: C₂₈H₃₂N₄O₂S

Batch Molecular Weight: 488.64

Physical Appearance: White solid

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.

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