

**Product Name:** NNC 26-9100

**Catalog No.:** 2440

**Batch No.:** 3

CAS Number: 199522-35-5

IUPAC Name: 1-[3-[N-(5-Bromopyridin-2-yl)-N-(3,4-dichlorobenzyl)amino]propyl]-3-[3-(1H-imidazol-4-yl)propyl]thiourea

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>22</sub>H<sub>25</sub>N<sub>6</sub>Cl<sub>2</sub>SBr·¼H<sub>2</sub>O

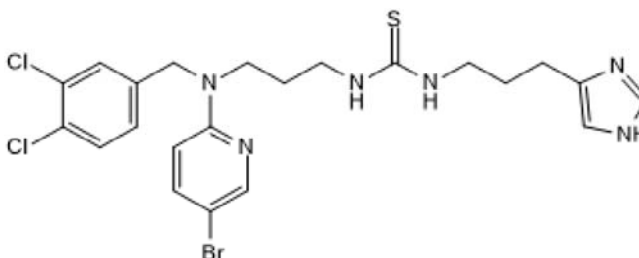
**Batch Molecular Weight:** 560.85

**Physical Appearance:** White solid

**Solubility:** DMSO to 50 mM  
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.63 (10% MeOH, 0.25% NH<sub>4</sub>OH in EtOAc)

**HPLC:** Shows 99.3% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	47.11	4.58	14.98
Found	47.08	4.52	14.64

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**Description:**

NNC 26-9100 is a somatostatin sst<sub>4</sub> receptor agonist that displays > 100-fold selectivity over sst<sub>2</sub> receptors (K<sub>i</sub> values are 6 and 621 nM for sst<sub>4</sub> and sst<sub>2</sub> receptors respectively). Potently inhibits forskolin-induced cAMP accumulation (EC<sub>50</sub> = 26 nM).

**Physical and Chemical Properties:**

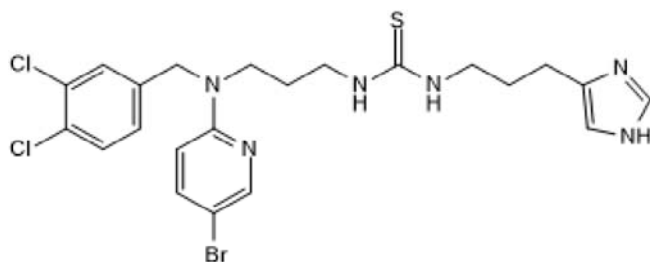
Batch Molecular Formula: C<sub>22</sub>H<sub>25</sub>N<sub>6</sub>Cl<sub>2</sub>SBr.¼H<sub>2</sub>O

Batch Molecular Weight: 560.85

Physical Appearance: White solid

**Minimum Purity:** ≥99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 50 mM

ethanol to 50 mM

By NMR this product contains 0.25 molar equivalents of ethanol.

**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:**

Liu *et al* (1999) 2-pyridylthioureas: novel nonpeptide somatostatin agonists with SST4 selectivity. *Curr.Pharm.Des.* **5** 255. PMID: 10101224.

Liu *et al* (1998) Nonpeptide somatostatin agonists with sst4 selectivity: synthesis and structure-activity relationships of thioureas. *J.Med.Chem.* **41** 4693. PMID: 9822540.

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