

Product Name: BX 471

Catalog No.: 3496

Batch No.: 3

CAS Number: 217645-70-0

IUPAC Name: (2R)-1-[[2-[(Aminocarbonyl)amino]-4-chlorophenoxy]acetyl]-4-[(4-fluorophenyl)methyl]-2-methylpiperazine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₄ClFN₄O₃·1¼H₂O

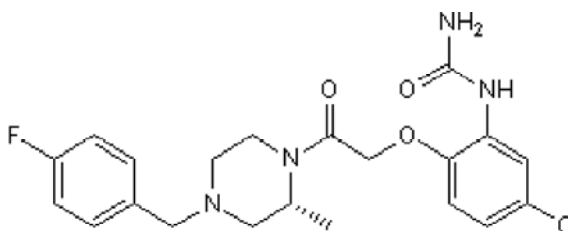
Batch Molecular Weight: 457.41

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

Chiral HPLC: Shows 99.87% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 55.14 | 5.84 | 12.25 |
| Found | 54.91 | 5.92 | 12.36 |

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

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Description:

Potent, selective non-peptide CCR1 antagonist ($K_i = 1$ nM for human CCR1). Exhibits 250-fold selectivity for CCR1 over CCR2, CCR5 and CXCR4. Inhibits MIP- α /CCL3-induced intracellular Ca^{2+} mobilization. Orally active; effectively reduces disease severity in a rat model of multiple sclerosis. Decreases renal fibrosis in a mouse model of obstructive nephropathy.

Physical and Chemical Properties:

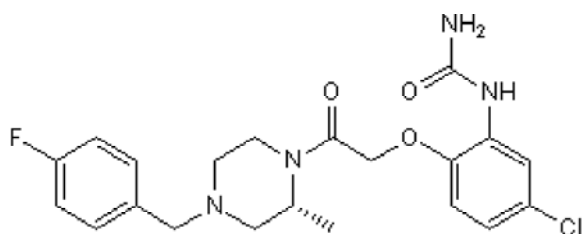
Batch Molecular Formula: $C_{21}H_{24}ClFN_4O_3 \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 457.41

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 50 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:

Furuichi et al (2008) Chemokine receptor CCR1 regulates inflammatory cell infiltration after renal ischemia-reperfusion injury. *J.Immunol.* **181** 8670. PMID: 19050287.

Anders (2002) A chemokine receptor CCR-1 antagonist reduces renal fibrosis after unilateral ureter ligation. *J.Clin.Invest.* **109** (2) 251. PMID: 11805137.

Liang (2000) Identification and characterization of a potent, selective, and orally active antagonist of the CC chemokine receptor-1. *J.Biol.Chem.* **275** (25) 19000. PMID: 10748002.

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