

Product Name: (±)-NBI 74330

Catalog No.: 4528

Batch No.: 5

CAS Number: 473722-68-8

IUPAC Name: *N*-1-[(3-4(-Ethoxyphenyl)-3,4-dihydro-4-oxopyrido[2,3-*d*]pyrimidin-2-yl)ethyl]-4-fluoro-*N*-(3-pyridinylmethyl)-3-(trifluoromethyl)benzeneacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₂H₂₇F₄N₅O₃ · ½H₂O

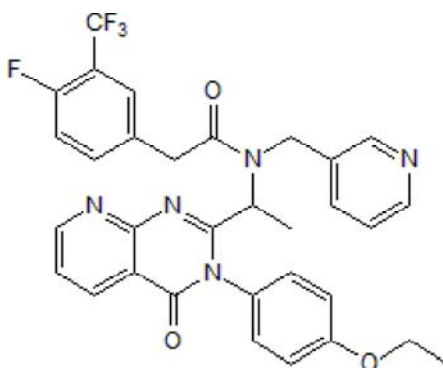
Batch Molecular Weight: 614.59

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.54	4.59	11.4
Found	62.27	4.55	11.23

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Description:

Potent and selective CXCR3 antagonist; potently inhibits ¹²⁵I-CXCL10 binding to CXCR3 (pK_i = 8.13). Inhibits calcium mobilization in response to CXCL11 and CXCL10 in RBL cells. Exhibits no significant effect on chemotaxis induced by CXCR4 or CCR7. Displays a five-fold greater affinity for CXCR3 than (±)-AMG 487. This product is racemic.

Physical and Chemical Properties:

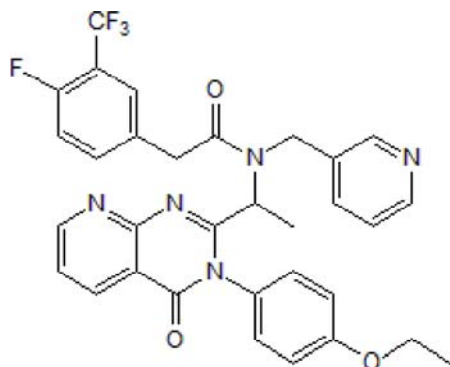
Batch Molecular Formula: C₃₂H₂₇F₄N₅O₃·½H₂O

Batch Molecular Weight: 614.59

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM

This compound is racemic.

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:

Verziji et al (2008) Noncompetitive antagonism and inverse agonism as mechanism of action of nonpeptidergic antagonists at primate and rodent CXCR3 chemokine receptors. *J.Pharmacol.Exp.Ther.* **325** 544. PMID: 18270317.

Storelli et al (2007) Synthesis and structure-activity relationships of 3H-quinazolin-4-ones and 3H-pyrido[2,3-*d*]pyrimidin-4-ones as CXCR3 receptor antagonists. *Arch.Pharm.* **340** 281. PMID: 17562560.

Heise et al (2005) Pharmacological characterization of CXC chemokine receptor 3 ligands and a small molecule antagonist. *J.Pharmacol.Exp.Ther.* **313** 1263. PMID: 15761110.

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