

Product Name: (±)-AMG 487

Catalog No.: 4487

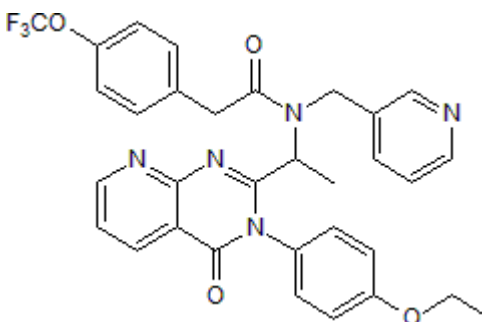
Batch No.: 3

CAS Number: 947536-03-0

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₂H₂₈F₃N₅O₄·¼H₂O
Batch Molecular Weight: 608.09
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.68 (Chloroform:MeOH:NH₄OH [10:1:0.1])
HPLC: Shows 99% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.21	4.72	11.52
Found	63.25	4.77	11.52

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

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Description:

Antagonist of CXCR3; inhibits binding of ¹²⁵I-IP-10 and ¹²⁵I-ITAC to CXCR3 (IC₅₀ values are 8.0 and 8.2 nM respectively). Inhibits CXCR3-mediated cell migration by the chemokines IP-10, ITAC and MiG in vitro (IC₅₀ values are 8, 15 and 36 nM respectively). Also shown to inhibit lung metastasis in a mouse model of metastatic breast cancer.

Physical and Chemical Properties:

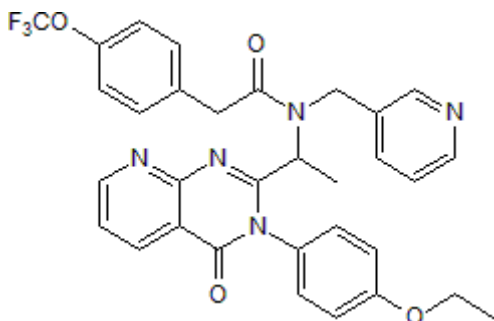
Batch Molecular Formula: C₃₂H₂₈F₃N₅O₄·½H₂O

Batch Molecular Weight: 608.09

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 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:

Cambien *et al* (2009) Organ-specific inhibition of metastatic colon carcinoma by CXCR3 antagonism. *Br.J.Cancer* **100** 1755. PMID: 19436305.

Johnson *et al* (2007) Discovery and optimization of a series of quinazolinone-derived antagonists of CXCR3. *Bioorg.Med.Chem.Lett.* **17** 3339. PMID: 17448658.

Walser *et al* (2006) Antagonism of CXCR3 inhibits lung metastasis in a murine model of metastatic breast cancer. *Cancer Res.* **66** 7701. PMID: 16885372.

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