

Product Name: VUF 11207 fumarate

Catalog No.: 4780

Batch No.: 1

CAS Number: 1785665-61-3

IUPAC Name: *N*-[(2*E*)-3-(2-Fluorophenyl)-2-methyl-2-propen-1-yl]-3,4,5-trimethoxy-*N*-[2-(1-methyl-2-pyrrolidiny)ethyl]benzamide fumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₃₅FN₂O₄·C₄H₄O₄·H₂O

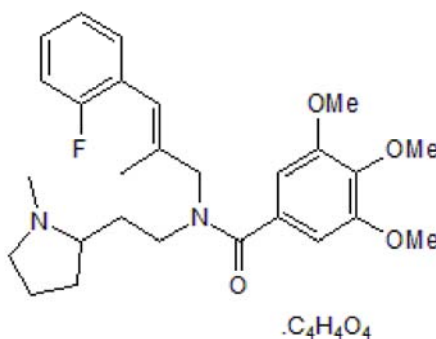
Batch Molecular Weight: 604.67

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Chloroform:Methanol:Ammonia soln. [95:5:0.1])

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.58	6.83	4.63
Found	61.57	6.48	4.63

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

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Description:

Potent ACKR3 (CXCR7) chemokine receptor agonist ($EC_{50} = 1.6$ nM). Induces recruitment of β -arrestin to CXCR7 in HEK293-CXCR7 cells.

Physical and Chemical Properties:

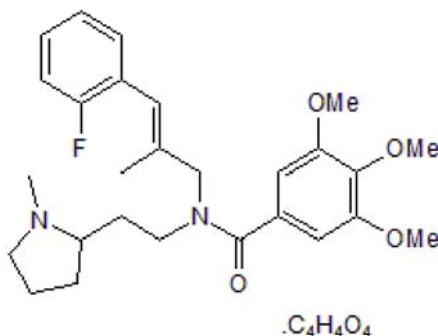
Batch Molecular Formula: $C_{27}H_{35}FN_2O_4 \cdot C_4H_4O_4 \cdot H_2O$

Batch Molecular Weight: 604.67

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

CAUTION: This compound is hygroscopic and has been packed under inert atmosphere.

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ 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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Wijtmans *et al* (2012) Synthesis, modeling and functional activity of substituted styrene-amides as small-molecule CXCR7 agonists. *Eur.J.Med.Chem.* **51** 184. PMID: 22424612.

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