Product Name: VUF 11207 fumarate
Catalog No.: 4780
Batch No.: 1
CAS Number: 1785665-61-3
IUPAC Name: N-[(2E)-3-(2-Fluorophenyl)-2-methyl-2-propen-1-yl]-3,4,5-trimethoxy-N-[2-(1-methyl-2-pyrrolidinyl)ethyl]benzamide fumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{35}FN_2O_4.C_4H_4O_4.H_2O$
Batch Molecular Weight: 604.67
Physical Appearance: White solid
Solubility: water to 100 mM
DMSO to 100 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: $R_f = 0.4$ (Chloroform:Methanol:Ammonia soln. [95:5:0.1])
HPLC: Shows 98.4% purity
$^1$H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
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<tr>
<td>Hydrogen</td>
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<tr>
<td>Nitrogen</td>
<td>4.63</td>
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</table>
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**Description:**
Potent ACKR3 (CXCR7) chemokine receptor agonist ($EC_{50} = 1.6$ nM). Induces recruitment of $\beta$-arrestin to CXCR7 in HEK293-CXCR7 cells.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** $C_{22}H_{35}FN_{2}O_{4}$, $C_{15}H_{20}O_{4} \cdot H_{2}O$
- **Batch Molecular Weight:** 604.67
- **Physical Appearance:** White solid
- **Minimum Purity:** $\geq 98\%$
- **Batch Molecular Structure:**

![Molecular Structure Image]

**Storage:** Store at -20°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°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:**