1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $\text{C}_{33}\text{H}_{44}\text{N}_{6}\text{O}_{5} \cdot \frac{1}{2}\text{H}_{2}\text{O}$

Batch Molecular Weight: 613.76

Physical Appearance: White solid

Solubility: 1eq. HCl to 100 mM
DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:

![Molecular Structure Image]

2. ANALYTICAL DATA

TLC: $R_f = 0.65$ (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

Melting Point: Between 113 - 120°C

HPLC: Shows 100% purity

$^1$H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>64.6</td>
<td>64.55</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.39</td>
<td>7.35</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>13.7</td>
<td>13.63</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Others</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Product Information

Product Name: FR 139317
Catalog No.: 1210
Batch No.: 1

CAS Number: 142375-60-8
IUPAC Name: N-[N-[N-(Hexahydro-1H-azepin-1-yl)carbonyl]-L-leucyl]-1-methyl-D-tryptophyl]-3-(2-pyridinyl)-D-alanine

Description:
A highly potent and selective ET<sub>A</sub> endothelin receptor antagonist (K<sub>i</sub> values are 1 nM and 7.3 μM at ET<sub>A</sub> and ET<sub>B</sub> subtypes respectively). Active in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C<sub>33</sub>H<sub>44</sub>N<sub>6</sub>O<sub>5</sub>·½H<sub>2</sub>O
Batch Molecular Weight: 613.76
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Desiccate at +4°C

Solubility & Usage Info:
1eq. HCl to 100 mM
DMSO to 100 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: