Product Name: BMS 193885  
Catalog No.: 3242  
Batch No.: 2

CAS Number: 679839-66-8

IUPAC Name: 1,4-Dihydro-4-[[3-[4-(3-methoxyphenyl)-1-piperidinyl]propyl]amino]carbonyl]amino]phenyl]-2,6-dimethyl-3,5-pyridinedicarboxylic acid 3,5-dimethyl ester L-Lactate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{33}H_{42}N_{4}O_{6} \cdot C_{3}H_{6}O_{3} \cdot H_{2}O$

Batch Molecular Weight: 698.81

Physical Appearance: Pale yellow solid

Solubility: water to 20 mM  
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

TLC: $R_f = 0.48$ (Dichloromethane: Methanol: Ammonia soln. [90:9.5:0.5])

HPLC: Shows 99.5% purity

$^1$H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>61.88</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.21</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>8.02</td>
</tr>
</tbody>
</table>
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IUPAC Name: 1,4-Dihydro-4-[3-[4-[3-(3-methoxyphenyl)-1-piperidinyl]propyl]amino]carbonyl]amino]phenyl]-2,6-dimethyl-3,5-pyridinedicarboxylic acid 3,5-dimethyl ester L-Lactate

Description:
Potent, competitive neuropeptide (NPY) Y₁ antagonist (Kᵢ = 3.3 nM, IC₅₀ = 5.9 nM) that displays > 47, > 100, > 160, > 160 and > 160-fold selectivity over σ₁, α₁, Y₂, Y₄ and Y₅ receptors respectively. Reduces food intake and body weight via central Y₁ inhibition and is brain penetrant.

Physical and Chemical Properties:
Batch Molecular Formula: C₃₅H₄₅N₄O₁₀C₂H₆O₃.H₂O
Batch Molecular Weight: 698.81
Physical Appearance: Pale yellow solid
Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate at RT
CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:
water to 20 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: