1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  \[ \text{C}_{27}\text{H}_{31}\text{N}_{5}\text{O}_{3}\cdot 1.5\text{CF}_{3}\text{CO}_{2}\text{H} \]
Batch Molecular Weight:  644.6
Physical Appearance:  Off-white solid
Solubility:  water to 10 mM with sonication
            DMSO to 100 mM
Storage:  Store at -20°C

2. ANALYTICAL DATA

HPLC:  Shows 98.2% purity

\(^1\text{H} \text{NMR:} \)  Consistent with structure

Mass Spectrum:  Consistent with structure
Optical Rotation:  \([\alpha]_D = +18.2 \) (Concentration = 1, Solvent = Water)

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
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</thead>
<tbody>
<tr>
<td>C</td>
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<tr>
<td>H</td>
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<td>4.82</td>
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<tr>
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<td>11.05</td>
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</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: BIBP 3226 trifluoroacetate
Catalog No.: 2707
Batch No.: 3

IUPAC Name: N-[(1R)-4-[(Aminoiminomethyl)amino]-1-[[4-hydroxyphenyl)methyl]amino]carbonyl]butyl-α-phenylbenzeneacetamide

Description:
Mixed non-peptide neuropeptide Y (NPY Y1) and neuropeptide FF (NPFF) receptor antagonist (Kᵢ values are 1.1, 79, 108, > 1000, > 1000 and >1000 for rNPY Y₁, hNPFF₂, rNPFF, rNPY Y₂, rNPY Y₄ and rNPY Y₅ respectively). Produces an anxiogenic-like effect in rats following i.c.v. administration.

Physical and Chemical Properties:
Batch Molecular Formula: C₃₂H₃₁N₁₀O₈.1.5CF₃CO₂H
Batch Molecular Weight: 644.6
Physical Appearance: Off-white solid
Minimum Purity: >98%

Solubility & Usage Info:
- water to 10 mM with sonication
- DMSO to 100 mM

When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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.

Other Information:
This product is sold as a TFA salt. The exact stoichiometry of the salt is batch dependant.

References: