

Product Name: BIBN 4096

Catalog No.: 4561

Batch No.: 8

CAS Number: 204697-65-4

IUPAC Name: 1-[3,5-Dibromo-*N*-[[4-(1,4-dihydro-2-oxo-3(2*H*)-quinazoliny)-1-piperidiny]carbonyl]-*D*-tyrosyl-*L*-lysyl]-4-(4-pyridinyl)-piperazine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₈H₄₇Br₂N₉O₅·2¾H₂O

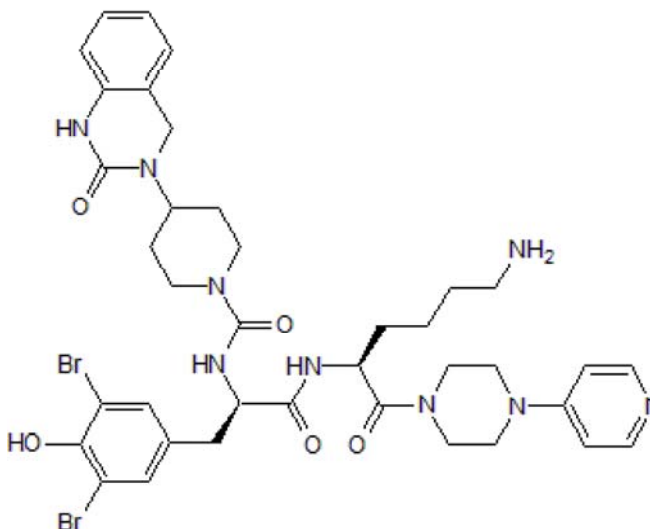
Batch Molecular Weight: 919.19

Physical Appearance: White solid

Solubility: DMSO to 50 mM
2eq.HCl to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -27.9 (Concentration = 1, Solvent = DMSO)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.65	5.76	13.71
Found	49.5	5.47	13.67

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

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Description:

Potent and selective CGRP receptor antagonist (IC₅₀ values are 0.03 and 6.4 nM for human and rat CGRP receptors respectively). Displays high affinity for human CGRP receptors (K_i = 14.4 pM); exhibits no significant affinity for 75 other receptors.

Physical and Chemical Properties:

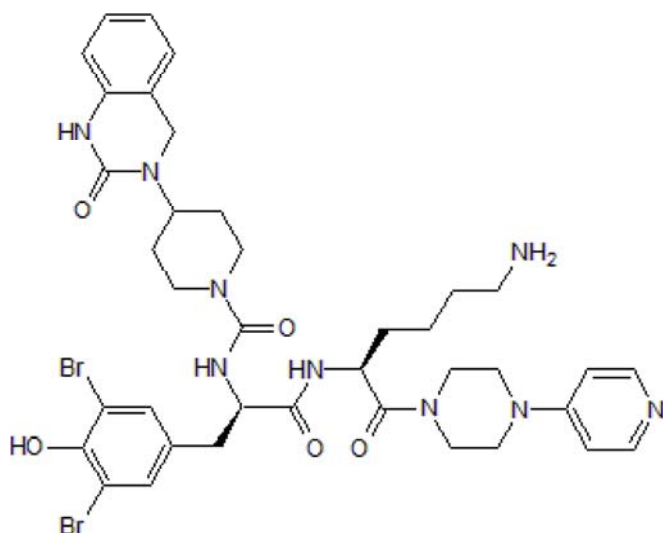
Batch Molecular Formula: C₃₈H₄₇Br₂N₉O₅·2¾H₂O

Batch Molecular Weight: 919.19

Physical Appearance: White solid

Minimum Purity: >95%

Batch Molecular Structure:



References:

Rudolf et al (2005) Development of human calcitonin gene-related peptide (CGRP) receptor antagonists. 1. Potent and selective small molecule CGRP antagonists. 1-[N²-[3,5-Dibromo-N-[[4-(3,4-dihydro-2(1H)-oxoquinazolin-3-yl)-1-piperidiny]carbonyl]-D-tyrosyl]-L-lysyl]-4-(4-pyridinyl)piperazine: the first CGRP antagonist for clinical trials in acute migraine. *J.Med.Chem.* **48** 5921. PMID: 16161996.

Doods et al (2000) Pharmacological profile of BIBN4096BS, the first selective small molecule CGRP antagonist. *Br.J.Pharmacol.* **129** 420. PMID: 10711339.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM

2eq.HCl to 50 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.

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