

**Product Name:** BIBN 4096

**Catalog No.:** 4561

**Batch No.:** 3

**CAS Number:** 204697-65-4

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>38</sub>H<sub>47</sub>Br<sub>2</sub>N<sub>9</sub>O<sub>5</sub>·H<sub>2</sub>O

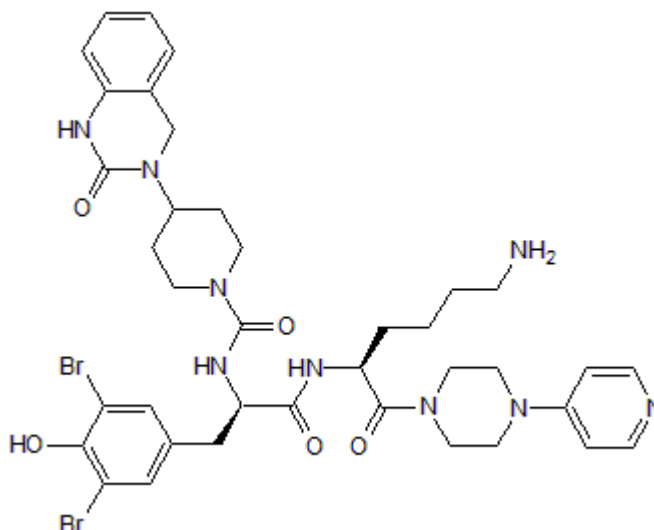
**Batch Molecular Weight:** 887.67

**Physical Appearance:** Off-white solid

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

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.17 (Dichloromethane:Methanol [90:10] +4 drops NH<sub>4</sub>OH)

**HPLC:** Shows 97.1% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = -27 (Concentration = 1, Solvent = DMSO)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	51.42	5.56	14.2
Found	51.04	5.65	13.98

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

Tocris Bioscience is an R&D Systems company  
 USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373  
[www.RnDSystems.com](http://www.RnDSystems.com)

**R&D**  
SYSTEMS®

**Product Name:** BIBN 4096

**Catalog No.:** 4561

**Batch No.:** 3

**CAS Number:** 204697-65-4

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

**Description:**

Potent and selective CGRP receptor antagonist (IC<sub>50</sub> values are 0.03 and 6.4 nM for human and rat CGRP receptors respectively). Displays high affinity for human CGRP receptors (K<sub>i</sub> = 14.4 pM); exhibits no significant affinity for 75 other receptors.

**Physical and Chemical Properties:**

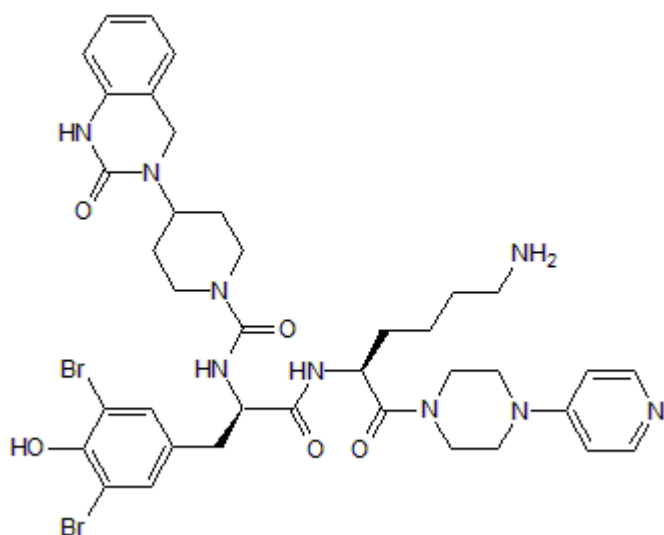
Batch Molecular Formula: C<sub>38</sub>H<sub>47</sub>Br<sub>2</sub>N<sub>9</sub>O<sub>5</sub>·H<sub>2</sub>O

Batch Molecular Weight: 887.67

Physical Appearance: Off-white solid

**Minimum Purity:** >96%

**Batch Molecular Structure:**



**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.

**References:**

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

**Rudolf et al (2005)** Development of human calcitonin gene-related peptide (CGRP) receptor antagonists. 1. Potent and selective small molecule CGRP antagonists. 1-[N<sup>2</sup>-[3,5-Dibromo-N-[[4-(3,4-dihydro-2(1H)-oxoquinazolin-3-yl)]-1-piperidinyl]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.

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

Tocris Bioscience is an R&D Systems company  
USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373  
[www.RnDSystems.com](http://www.RnDSystems.com)

