bio-techne
TOCRIS

Print Date: Jun 28th 2023

Certificate of Analysis

www.tocris.com

Product Name: **BIBN 4096** **Catalog No.: 4561** **Batch No.: 9**

CAS Number: 204697-65-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{38}H_{47}Br_2N_9O_5.2¼H_2O$

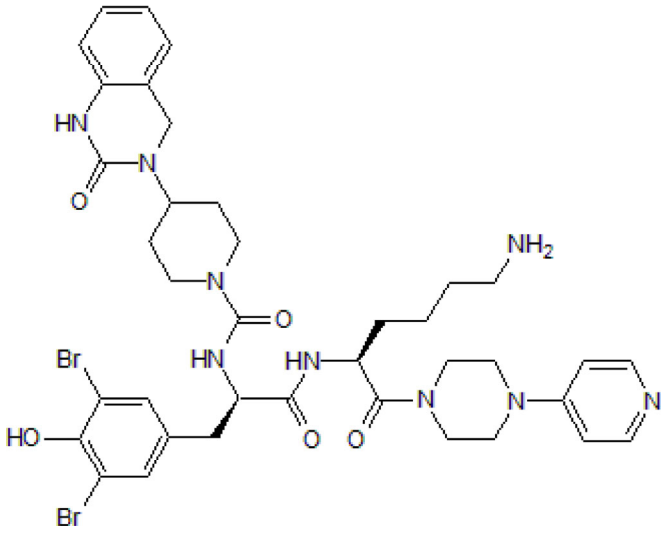
Batch Molecular Weight: 910.18

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 97.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -26.3 (Concentration = 1, Solvent = DMSO)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.15	5.7	13.85
Found	49.76	5.67	13.62

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Name: **BIBN 4096** **Catalog No.: 4561** **9**

CAS Number: 204697-65-4

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

Description:

BIBN 4096 is a potent and selective CGRP receptor antagonist (IC_{50} 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. BIBN 4096 improves pain symptoms in a mouse migraine model.

Physical and Chemical Properties:

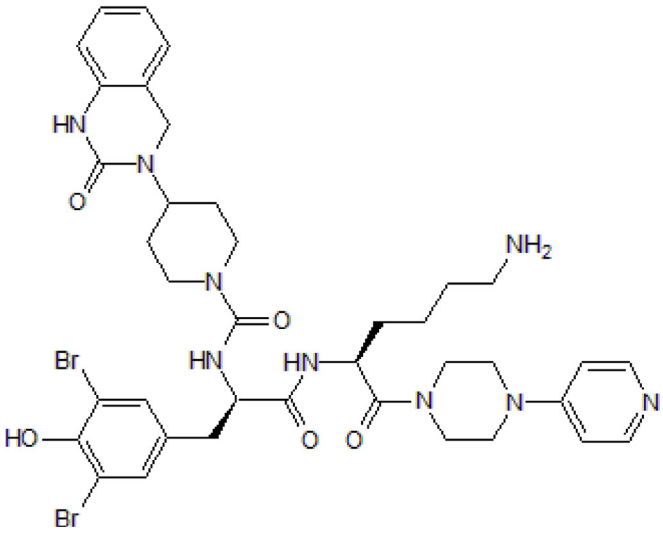
Batch Molecular Formula: $C_{38}H_{47}Br_2N_9O_5.2¼H_2O$

Batch Molecular Weight: 910.18

Physical Appearance: White solid

Minimum Purity: ≥95%

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Prado *et al* (2021) TREK channel activation suppresses migraine pain phenotype. iScience ***24*** 102961. PMID: 34458705.

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- piperidinyl 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.