

Certificate of Analysis

Print Date: Sep 25th 2023

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Product Name: (Z)-Pugnac Catalog No.: 3384 Batch No.: 9

CAS Number: 132489-69-1

IUPAC Name: O-(2-Acetamido-2-deoxy-D-glucopyranosylidene)amino-Z-N-phenylcarbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{19}N_3O_7.1\frac{1}{2}H_2O$

Batch Molecular Weight: 380.35

Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +61.8$ (Concentration = 0.2, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 47.37 5.83 11.05 Found 46.94 5.71 11.02



Product Information

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IUPAC Name: O-(2-Acetamido-2-deoxy-D-glucopyranosylidene)amino-Z-N-phenylcarbamate

Description:

(Z)-Pugnac is an O-GlcNAc-β-N-acetylglucosaminidase (O-GlcNAcase) and β-hexosaminidase inhibitor (K_i values are 46 and 36 nM respectively) that increases O-GlcNAc levels ~ 2-fold in HT29 cells. Z-linked isomer is more potent than the E isomer.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₅H₁₉N₃O₇.1½H₂O

Batch Molecular Weight: 380.35 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

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. *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:

Perreira et al (2006) Inhibition of O-GlcNAcase by PUGNAc is dependent upon the oxime stereochemistry. Bioorg.Med.Chem. **14** 837. PMID: 16214344.

Macauley et al (2005) O-GlcNAcase uses substrate-assisted catalysis. J.Biol.Chem. 280 25313. PMID: 15795231.

Dong and Hart (1994) Purification and characterization of an O-GlcNAc selective *N*-acetyl-β-D-glucosaminidase from rat spleen cytosol. J.Biol.Chem. **269** 19321. PMID: 8034696.

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