



Certificate of Analysis

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Product Name: BTT 3033 Catalog No.: 4724 Batch No.: 1

CAS Number: 1259028-99-3

IUPAC Name: 1-(4-Fluorophenyl)-N-methyl-N-[4[[(phenylamino)carbonyl]amino]phenyl]-1H-pyrazole-4-sulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{20}FN_5O_3S$

Batch Molecular Weight: 465.5

Physical Appearance: White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.52$ (Chloroform:Methanol [97:3])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 59.34 4.33 15.04 Found 59.31 4.3 15.1

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

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Product Information

Print Date: Nov 8th 2021

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IUPAC Name: 1-(4-Fluorophenyl)-N-methyl-N-[4[[(phenylamino)carbonyl]amino]phenyl]-1H-pyrazole-4-sulfonamide

Description:

BTT 3033 is a selective inhibitor of integrin $\alpha_2\beta_1$ (EC $_{50}$ = 130 nM for $\alpha_2\beta_1$ binding to collagen I). Binds to the α_2 I domain. Exhibits selectivity for $\alpha_2\beta_1$ over integrins $\alpha_3\beta_1$, $\alpha_4\beta_1$, $\alpha_5\beta_1$ and α_v . BTT 3033 inhibits platelet aggregation to collagen I coated capillaries under flow and inhibits binding of α_2 -expressing CHO cells to collagen I under shear stress conditions. Neurogenic and thromboxane A $_2$ -induced human prostate smooth muscle contraction are also inhibited by BTT 3033. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C23H20FN5O3S

Batch Molecular Weight: 465.5 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at +4°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. 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:

Li et al (2021) Phosphoproteomics identifies potential downstream targets of the integrin $\alpha 2\beta 1$ inhibitor BTT-3033 in prostate stromal cells. Ann.Transl.Med. 9 1380. PMID: 34733932.

Nissinen et al (2012) Novel a2ß1 integrin inhibitors reveal that integrin binding to collagen under shear stress conditions does not require receptor preactivation. J.Cell Biol. **287** 44694. PMID: 23132859.

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