

**Product Name:** BTT 3033

**Catalog No.:** 4724

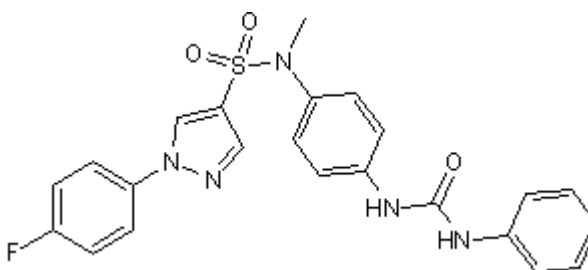
**Batch No.:** 1

CAS Number: 1259028-99-3

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

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>23</sub>H<sub>20</sub>FN<sub>5</sub>O<sub>3</sub>S  
**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<sub>f</sub> = 0.52 (Chloroform:Methanol [97:3])  
**HPLC:** Shows 99.8% purity  
**<sup>1</sup>H 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

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**Description:**

Selective inhibitor of integrin  $\alpha_2\beta_1$  ( $EC_{50}$  = 130 nM for  $\alpha_2\beta_1$  binding to collagen I). Binds to the  $\alpha_2$ I domain. Exhibits selectivity for  $\alpha_2\beta_1$  over integrins  $\alpha_3\beta_1$ ,  $\alpha_4\beta_1$ ,  $\alpha_5\beta_1$  and  $\alpha_v$ . Inhibits platelet aggregation to collagen I coated capillaries under flow. Also inhibits binding of  $\alpha_2$ -expressing CHO cells to collagen I under shear stress conditions.

**Physical and Chemical Properties:**

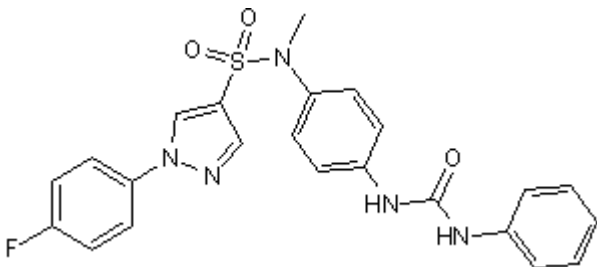
Batch Molecular Formula: C<sub>23</sub>H<sub>20</sub>FN<sub>5</sub>O<sub>3</sub>S

Batch Molecular Weight: 465.5

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Nissinen et al** (2012) Novel  $\alpha_2\beta_1$  integrin inhibitors reveal that integrin binding to collagen under shear stress conditions does not require receptor preactivation. *J. Cell Biol.* **287** 44694. PMID: 23132859.

**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.

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