

## Certificate of Analysis

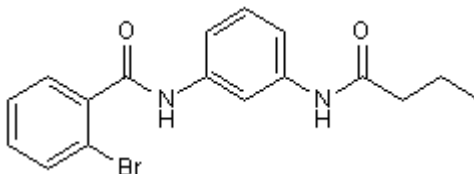
[www.tocris.com](http://www.tocris.com)

**Product Name:** ML 161  
**CAS Number:** 423735-93-7  
**IUPAC Name:** 2-Bromo-N-[3-[(1-oxobutyl)amino]phenyl]benzamide

**Catalog No.:** 4570 **Batch No.:** 1

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>17</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 361.23  
**Physical Appearance:** Brown solid  
**Solubility:** DMSO to 100 mM  
ethanol to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 99.1% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	56.53	4.74	7.76
Found	56.46	4.78	7.84

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

## Product Information

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### Description:

Inhibitor of protease-activated receptor 1 (PAR<sub>1</sub>)-mediated platelet activation (IC<sub>50</sub> = 0.26 µM for the inhibition of platelet P-selectin expression on human platelets). Thought to act allosterically. Also inhibits thrombin-induced platelet activation.

### Physical and Chemical Properties:

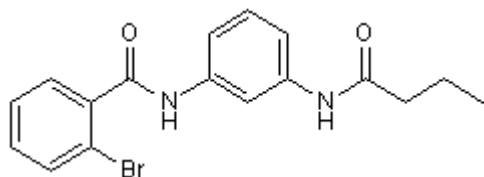
Batch Molecular Formula: C<sub>17</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>2</sub>

Batch Molecular Weight: 361.23

Physical Appearance: Brown solid

**Minimum Purity:** >98%

### Batch Molecular Structure:



**Storage:** Store at +4°C

### Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

**Dockendorff et al** (2012) Discovery of 1,3-diaminobenzenes as selective inhibitors of platelet activation at the PAR1 receptor. ACS Med.Chem.Lett. **3** 232. PMID: 22408714.

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