TOCRIS b i o s c i e n c e

Certificate of Analysis

Print Date: Aug 9th 2012

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Product Name: ML 161

Catalog No.: 4570 Batch No.: 1

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

Storage: Batch Molecular Structure: C₁₇H₁₇BrN₂O₂ 361.23 Brown solid DMSO to 100 mM ethanol to 100 mM Store at +4°C

Br

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis: Shows 99.1% purity Consistent with structure Consistent with structure

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

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Product Information

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Description:

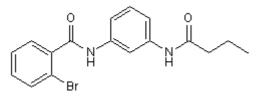
Inhibitor of protease-activated receptor 1 (PAR₁)-mediated platelet activation ($IC_{50} = 0.26 \ \mu M$ for the inhibition of platelet P-selectin expression on human platelets). Thought to act allosterically. Also inhibits thrombin-induced platelet activation.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₇BrN₂O₂ 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 $45-60^{\circ}$ 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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