

Certificate of Analysis

Print Date: Jan 14th 2016 **WWW.tocris.com**

Product Name: NSC 405020 Catalog No.: 4902 Batch No.: 1

CAS Number: 7497-07-6

IUPAC Name: 3,4-Dichloro-*N*-(1-methylbutyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{15}CI_2NO$

Batch Molecular Weight: 260.16

Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:

a Q N

2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.4 5.81 5.38

Found 55.42 5.74 5.71



Product Information

Print Date: Jan 14th 2016

www.tocris.com

Product Name: NSC 405020 Catalog No.: 4902 Batch No.: 1

CAS Number: 7497-07-6

IUPAC Name: 3,4-Dichloro-*N*-(1-methylbutyl)benzamide

Description:

Membrane type-1 matrix metalloproteinase (MT1-MMP) inhibitor ($IC_{50} > 100 \mu mol/L$). Directly interacts with the hemopexin domain (PEX) of MT1-MMP, affecting homodimerization and repressing its pro-tumorigenic activity in vivo. Displays no effect on the catalytic activity of MT1-MMP or MMP-2.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₂H₁₅Cl₂NO Batch Molecular Weight: 260.16 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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:

Remacle et al (2012) Novel MT1-MMP small-molecule inhibitors based on insights into hemopexin domain function in tumor growth. Cancer Res. **72** 2339. PMID: 22406620.