

Certificate of Analysis

www.tocris.com

Print Date: Jan 14th 2016

Product Name: ML 281 Catalog No.: 4880 Batch No.: 1

CAS Number: 1404437-62-2

IUPAC Name: N-[2-(3,4-Dihydro-3-oxo-2-quinoxalinyl)-4-(1-methylethyl)phenyl]-2-thiophenecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{19}N_3O_2S$

Batch Molecular Weight: 389.47

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

ethanol to 10 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.85 4.92 10.79 Found 67.89 4.89 10.78



Product Information

Print Date: Jan 14th 2016

www.tocris.com

Product Name: ML 281 Catalog No.: 4880 Batch No.: 1

CAS Number: 1404437-62-2

IUPAC Name: N-[2-(3,4-Dihydro-3-oxo-2-quinoxalinyl)-4-(1-methylethyl)phenyl]-2-thiophenecarboxamide

Description:

Inhibitor of the serine/threonine kinase STK33 ($IC_{50} = 14 \text{ nM}$). Exhibits >700-fold selectivity for STK33 over the structurally related protein kinase A (PKA); also exhibits 550-fold selectivity over Aurora kinase B.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₂H₁₉N₃O₂S Batch Molecular Weight: 389.47 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

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:

Weiwer et al (2012) A potent and selective quinoxaline-based STK33 inhibitor does not show synthetic lethality in KRAS-dependent cells. ACS Med.Chem.Lett. 3 1034. PMID: 23256033.