



Certificate of Analysis

www.tocris.com

Product Name: (S)-Crizotinib Catalog No.: 6025 Batch No.: 1

CAS Number: 1374356-45-2

IUPAC Name: 3-[(1S)-1-(2,6-Dichloro-3-fluorophenyl)ethoxy]-5-[1-(4-piperidinyl)-1*H*-pyrazol-4-yl]-2-pyridinamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{22}CI_2FN_5O.14H_2O$

Batch Molecular Weight: 454.84

Physical Appearance: Off White solid
Solubility: DMSO to 50 mM

1eq. HCl to 20 mM with gentle warming

ethanol to 20 mM

Storage: Store at RT

Batch Molecular Structure:

$$\mathsf{F} \overset{\mathsf{CI}}{\longleftarrow} \overset{\mathsf{O}}{\longleftarrow} \overset{\mathsf{N}}{\longrightarrow} \overset{\mathsf{N}}{\longleftarrow} \overset{\mathsf{N}}{\longleftarrow} \mathsf{N} \mathsf{H}$$

2. ANALYTICAL DATA

HPLC: Shows >98.3% purity
Chiral HPLC: Shows 100% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.45 4.99 15.4 Found 55.44 4.84 15.32



Product Information

Print Date: Oct 7th 2016

www.tocris.com

Product Name: (S)-Crizotinib Catalog No.: 6025 Batch No.: 1

CAS Number: 1374356-45-2

IUPAC Name: 3-[(1S)-1-(2,6-Dichloro-3-fluorophenyl)ethoxy]-5-[1-(4-piperidinyl)-1H-pyrazol-4-yl]-2-pyridinamine

Description:

Potent MTH1 inhibitor ($IC_{50} = 72 \text{ nM}$). Induces DNA damage and disrupts nucleotide pool homeostasis in cancer cells. Also attenuates colony formation of KRAS-mutated PANC1 cells in vitro. Suppresses tumor growth ~50% in a colon cancer carcinoma xenograft model.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{21}H_{22}Cl_2FN_5O.$ 1/4 H_2O

Batch Molecular Weight: 454.84 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 50 mM

1eq. HCl to 20 mM with gentle warming

ethanol to 20 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc

References:

Huber et al (2014) Stereospecific targeting of MTH1 by (S)-crizotinib as an anticancer strategy. Nature 508 222. PMID: 24695225.