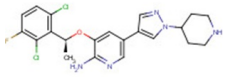
Data Sheet (Cat.No.T6357)

TargetMol
A DRUG SCREENING EXPERT

(S)-crizotinib

Chemical Properties



CAS No.:	1374356-45-2
Formula:	C21H22Cl2FN5O
Molecular Weight:	450.34
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	(S)-crizotinib（IC50 of 72 nM）, an effective MTH1 (NUDT1) inhibitor, is the (S)-enantiomer of crizotinib.
Targets(IC_{50})	MTH1: 72nM
Kinase Assay	MTH1 catalytic assay: Half-maximal inhibitory concentrations (IC50) are determined using a luminescence-based assay with some minor modifications. Briefly, serial dilutions of compounds are dissolved in assay buffer (100 mM Tris-acetate pH 7.5, 40 mM NaCl and 10 mM Mg(OAc)2 containing 0.005% Tween-20 and 2 mM dithiothreitol (DTT). Upon addition of MTH1 recombinant protein (final concentration 2 nM), plates are incubated on a plate shaker for 15 min at room temperature. After addition of the substrate dGTP (final concentration 100 µM), 8-oxo-dGTP (final concentration 13.2 µM), or 2-OH-dATP (final concentration 8.3 µM) the generation of pyrophosphate (PPi) as a result of nucleotide triphosphate hydrolysis by MTH1 is monitored over a time course of 15 min using the PPi Light Inorganic Pyrophosphate Assay kit. IC50 values are determined by fitting a dose-response curve to the data points using nonlinear regression analysis using the GraphPad Prism software.
Cell Research	One day before treatment, cells are seeded per well in six-well plates and incubated for 24 h. The next day DMSO (equal to highest amount of compound dilution, maximum 0.2%) or compounds in increasing concentrations were added and cells incubated at 37 °C, 5% CO2, for 7-10 days. After washing with PBS, cells are fixed with ice-cold methanol, stained with crystal violet solution (0.5% in 25% methanol) and left to dry overnight. For quantification of results, ultraviolet absorbance of crystal violet is determined at 595 nm following solubilisation by 70% ethanol. Data are analysed using nonlinear regression analysis using the GraphPad Prism software. (Only for Reference) Cell lines: PANC1 and SW480 cells
Animal Research	Animal Model: SW480 colon carcinoma xenograft mouse model.

Solubility Information

Solubility	1eq. HCl: 9 mg/mL (20 mM)) DMSO: 22.5 mg/mL (50 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.221 mL	11.103 mL	22.205 mL
5 mM	0.444 mL	2.221 mL	4.441 mL
10 mM	0.222 mL	1.11 mL	2.221 mL
50 mM	0.044 mL	0.222 mL	0.444 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Huber KV, et al. Nature. 2014 , 508(7495), 222-227.

2. Dai X, et al. (S)-crizotinib induces apoptosis in human non-small cell lung cancer cells by activating ROS independent of MTH1. J Exp Clin Cancer Res. 2017 Sep 7;36(1):120.

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