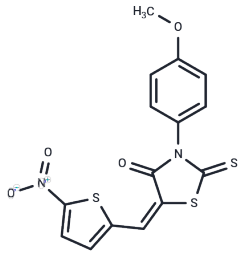
Data Sheet (Cat.No.T6800)

TargetMol

CCF642

Chemical Properties



CAS No. : 346640-08-2

Formula: C15H10N2O4S3

Molecular Weight: 378.45

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	CCF642 (AC1LYELL) is a novel PDI-inhibiting compound with antimyeloma activity.
Targets(IC50)	Others
In vitro	In vitro, CCF642 inhibits PDI reductase activity about 100-fold more potently than the structurally distinct established inhibitors PACMA 31 and LOC14. Computational modeling suggests a novel covalent binding mode in active-site CGHCK motifs. CCF642 causes acute ER stress in multiple myeloma cells accompanied by apoptosis-inducing calcium release[1].
In vivo	CCF642 displays potent efficacy in an aggressive syngeneic mouse model of multiple myeloma and prolongs the lifespan of C57BL/KaLwRij mice engrafted with 5TGM1-luc myeloma, an effect comparable to the first-line multiple myeloma therapeutic bortezomib[1].
Kinase Assay	Inhibition of CB-839 on rHu-GAC: The enzymatic activity is measured in assay buffer containing 50 mM Tris-Acetate pH 8.6, 150 mM K2HPO4 , 0.25 mM EDTA, 0.1 mg/mL bovine serum albumin, 1 mM DTT, 2 mM NADP+ and 0.01% Triton X-100. To measure inhibition, the inhibitor (prepared in DMSO) is first pre-mixed with glutamine and glutamate dehydrogenase (GDH) and reactions are initiated by the addition of rHu-GAC. Final reactions contains 2 nM rHu-GAC, 10 mM glutamine, 6 units/mL GDH and 2% DMSO. Generation of NADPH is monitored by fluorescence (Ex340/Em460 nm) every minute for 15 minutes on a SpectraMax M5e plate reader. Relative fluorescence units (RFU) are converted to units of NADPH concentration (μM) using a standard curve of NADPH. Each assay plate incorporates control reactions that monitores the conversion of glutamate (1 to 75 μM) plus NADP+ to α-ketoglutarate plus NADPH by GDH. Under these assay conditions, up to 75 μM glutamate is stoichiometrically converts to α-ketoglutarate/NADPH by GDH. Initial reaction velocities are calculated by fitting the first 5 minutes of each progress curve to a straight line. Inhibition curves are fitted to a four-parameter dose response equation of the form: % activity = Bottom + (Top-Bottom)/(1+10^((LogIC50-X)*HillSlope)).

Solubility Information

Solubility	DMSO: 11.11 mg/mL (29.36 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6424 mL	13.2118 mL	26.4236 mL
5 mM	0.5285 mL	2.6424 mL	5.2847 mL
10 mM	0.2642 mL	1.3212 mL	2.6424 mL
50 mM	0.0528 mL	0.2642 mL	0.5285 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

Vatolin S, et al. Cancer Res. 2016, 76(11):3340-50.
Yuan Z, Jing H, Deng Y, et al.P4HB maintains Wnt-dependent stemness in glioblastoma stem cells as a precision therapeutic target and serum marker.Oncogenesis.2024, 13(1): 42.

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