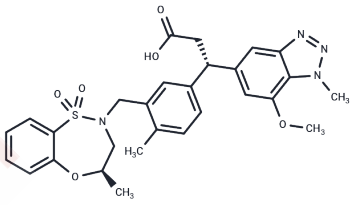
Data Sheet (Cat.No.T11758L)

KI696

Chemical Properties



CAS No. :	1799974-70-1
Formula:	C28H30N4O6S
Molecular Weight:	550.63
Storage:	Powder: -20°C for 3 years | In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.

Biological Description

Description	KI696 is a high-affinity probe that potently inhibits the interaction of Keap1 and NRF2.
Targets(IC50)	Nrf2
In vitro	KI696 displays high affinity for the KEAP1 Kelch domain with ITC Kd of 1.3 nM with the exception of the organic anion transporting polypeptide 1B1, the bile salt export pump BSEP and the phosphodiesterase PDE3A with an IC50 of 2.5 μM, 4.0 μM and 10 μM). KI696 causes an increase of NRF2 Nuclear Translocation in Normal Human Bronchial Epithelial cells and mRNA expression of the NRF2-dependent genes NQO1 and GCLM in NHBE cells transfected with the non-targeting siRNA in an NRF2-dependent manner[1].
In vivo	KI696 induces the expression of the Nqo1, Ho-1, Txnrd1, Srxn1, Gsta3, and Gclc genes in a dose-dependent manner with EC50s of 44.0, 25.7, 42.6, 33.8, 28.4, and 44.1 μmol/kg, respectively. KI696 attenuates ozone-Induced pulmonary inflammation and restores depletion of lung GSH levels. In rats, intravenous administration of KI696(10-50 μmol/kg) results in steady state compound concentrations in the blood of 407-1437 nM [1].

Solubility Information

Solubility	DMSO: 150 mg/mL (272.42 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 2 mg/mL (3.63 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.8161 mL	9.0805 mL	18.161 mL
5 mM	0.3632 mL	1.8161 mL	3.6322 mL
10 mM	0.1816 mL	0.9081 mL	1.8161 mL
50 mM	0.0363 mL	0.1816 mL	0.3632 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.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Davies TG, et al. Monoacidic Inhibitors of the Kelch-like ECH-Associated Protein 1: Nuclear Factor Erythroid 2-Related Factor 2 (KEAP1:NRF2) Protein-Protein Interaction with High Cell Potency Identified by Fragment-Based Discovery. J Med Chem. 2016 Apr 28;59(8):3991-4006.